



**Co-Optimization of
Fuels & Engines**

Co-Optima: Mixing-Controlled & Kinetically Controlled Compression-Ignition Combustion and Spray Research

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June 20, 2018

Project ID: FT056

SAND2018-4636PE

FY18 Vehicle Technologies Office Annual Merit Review

better fuels | better vehicles | sooner

Vehicle Technologies Office
Annual Merit Review
June 20, 2018

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Projects

Abbrev.	Description
ACI-F	Advanced Compression Ignition: Fuel Effects (Dec)
MCCI	Mixing-Controlled CI ¹ Combustion & Fuel Effects (Mueller)
SCO	Sprays/Combustion: Optical Imaging (Pickett)
SX	Sprays: X-Ray Imaging (Powell)
SS	Sprays: Simulation (Arienti)

¹CI = compression-ignition

Budget

Project	Lab	FY17 [\$k]	FY18 [\$k]
ACI-F	Sandia	175	170
MCCI	Sandia	864	250
SCO	Sandia	1150	250
SX	Argonne	150	150
SS	Sandia	-0-	190

Barriers*

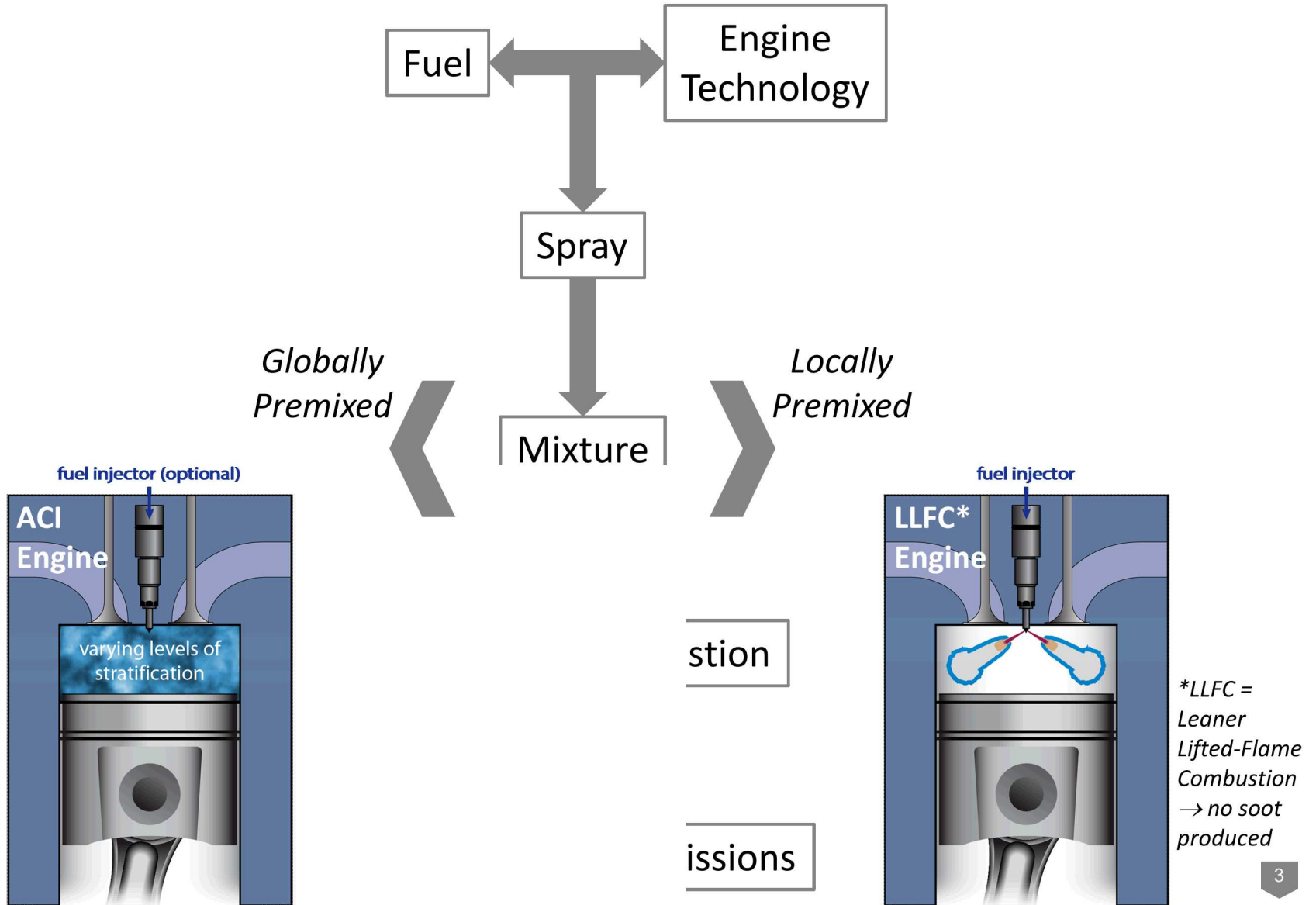
- Need improved combustion modes & understanding of fuel effects thereon
 - Advanced Compression Ignition
 - MCCI (a.k.a. clean-diesel) combustion
 - > Elevated nitrogen oxides and particulate emissions
 - > High costs of engine & aftertreatment systems
 - Sprays
 - > Lack of high-quality, fundamental data
 - > Inadequate predictive modeling capabilities

*from https://www.energy.gov/sites/prod/files/2018/03/f49/ACEC_TT_Roadmap_2018.pdf & <https://www.energy.gov/eere/vehicles/advanced-combustion-strategies>

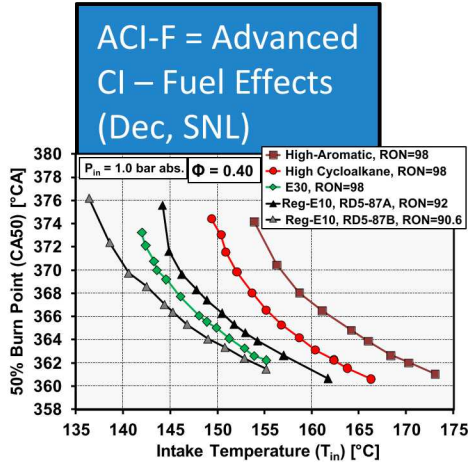
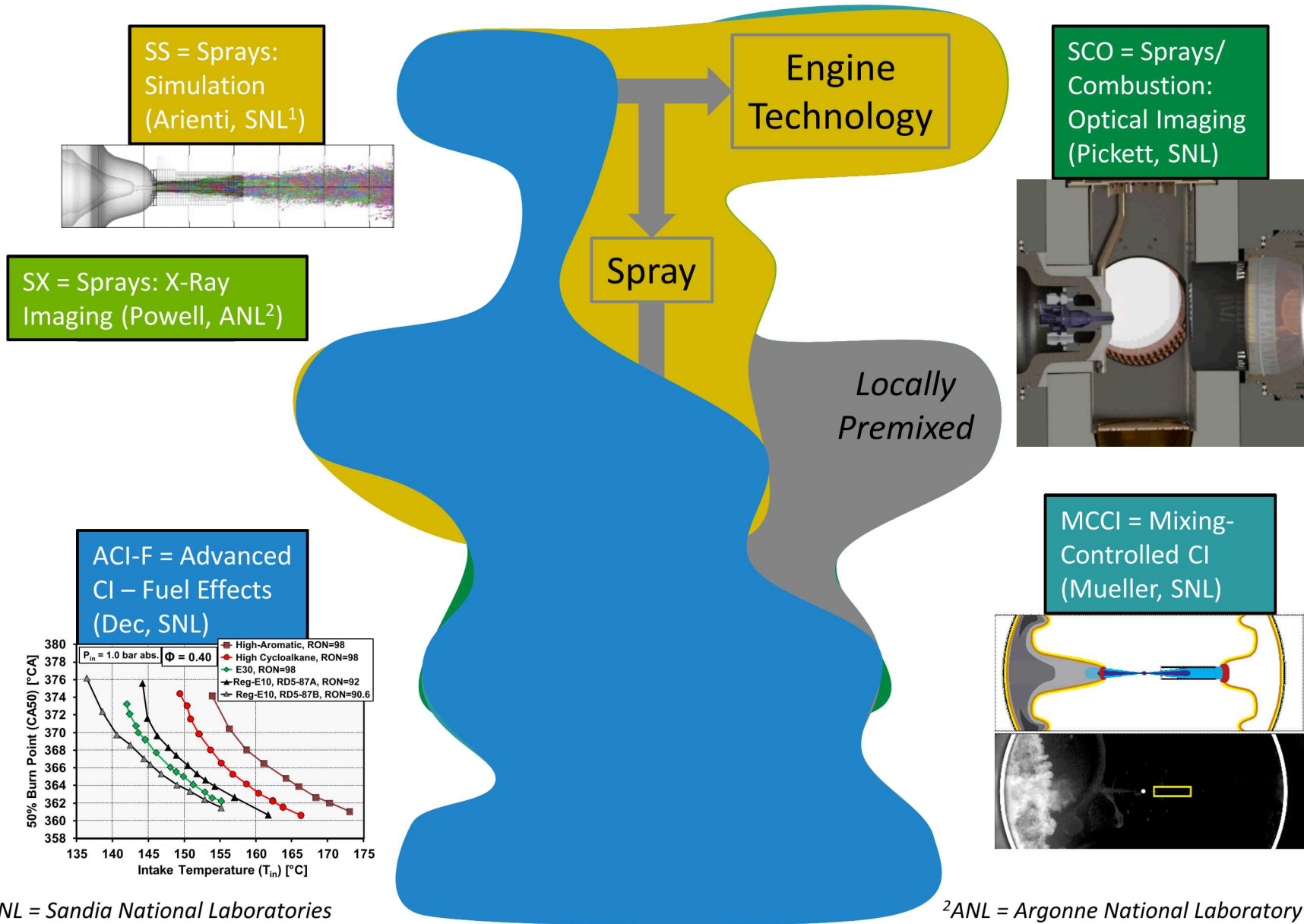
Timeline

Project	Start	End	% Compl.
ACI-F	10/2015	9/2018	83%
MCCI	10/2015	9/2018	83%
SCO	10/2015	9/2018	83%
SX	10/2015	9/2018	83%
SS	10/2017	9/2018	63%

Relevance



Approach



¹SNL = Sandia National Laboratories

²ANL = Argonne National Laboratory

Milestones



Mo/Yr	Proj.	Description of Milestone or Go/No-Go Decision	Status
Mar. '18	ACI-F	Complete data acquisition for the high-cycloalkane and E30 ¹ Co-Op ² fuels and compare w/ high-aromatic fuel & Reg. E10	✓
Sep. '18	ACI-F	Validation studies of LLNL ³ kinetic mechanisms & surrogates	Pending
Mar. '18	MCCI	1 st successful testing of ducted fuel inj. in the optical engine	✓
Sep. '18	MCCI	Optical-engine testing of two Coordinating Research Council Project AVFL ⁴ -18a diesel surrogate fuels	Pending funding
Mar. '18	SCO	Characterize GDI ⁵ spray behavior of Tier-3 selected fuels	Pending
Aug. '18	SCO	Complete high-throughput chamber and complete fuel-effect studies at relevant engine charge-gas conditions	Pending
Mar. '18	SX	Perform measurements of the near-nozzle fuel distribution resulting from iso-octane/ethanol/butanol blends under flash-boiling and non-flashing conditions	✓
Jun. '18	SS	Simulate fully unseated ECN ⁶ "Spray G" for two fuel blends	Pending

¹En = n vol% ethanol in gasoline; ²Co-Op = Co-Optima; ³LLNL = Lawrence Livermore National Laboratory; ⁴AVFL = Advanced Vehicles/Fuels/Lubricants; ⁵GDI = gasoline direct injection; ⁶ECN = Engine Combustion Network

Autoignition Characteristics of RON 98 Co-Optima Core Fuels and Regular E10 Gasolines



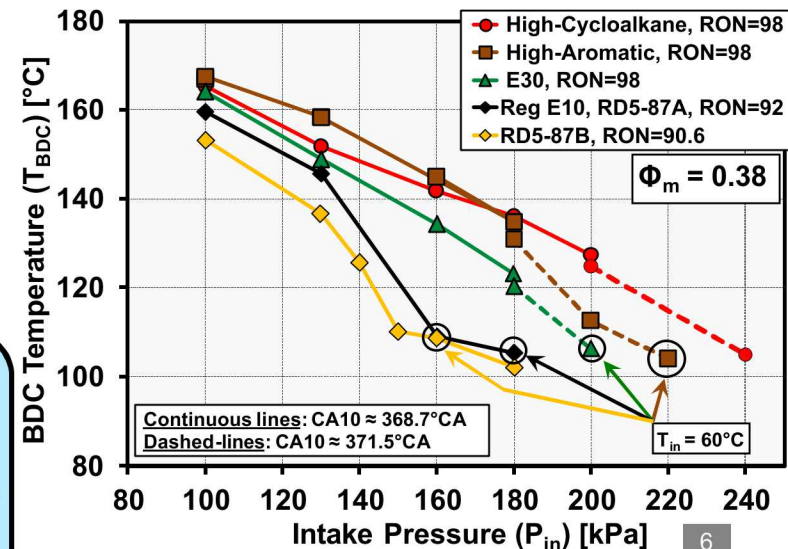
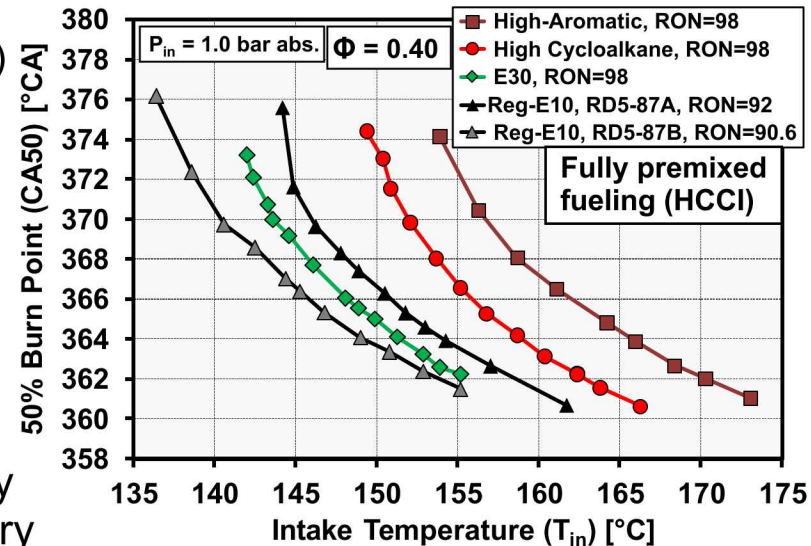
- Data-suites acquired for 3 additional fuels.
 - High-Cycloalkane Co-Optima fuel, RON 98
 - E30 Co-Op fuel, RON 98 (new data to correct error)
 - Regular E10: new batch, RD5-87B, **RON 90.5**

- $P_{in} = 1.0$ bar: The 3 Co-Optima fuels have very different reactivities, **despite all RON 98, $S \approx 11$**
 - Reactivity of E30 > Cycloalkane > Aromatic
 - Reactivity of E30 (RON 98) > RD5-87A (RON 92)

- Reactivity increases with boost:
 - Regular E10 fuels show large increase in reactivity for $P_{in} > 1.3$ bar \Rightarrow Due to onset of Low-T chemistry
 - RON-98 Co-Optima fuels show a more gradual increase in reactivity with boost, but \Rightarrow Significant differences between fuels
 - E30 is most reactive 98-RON Co-Opt fuel at all P_{in}
 - High-cycloalkane shows least reactivity increase with boost \Rightarrow Crosses the high-aromatic curve

- Cycloalkane should be very good for boosted SI
- RON, MON, & Octane Index (not shown) indicate some general trends, but aren't sufficient to specify fuel reactivity for lean well-mixed ACI (i.e. HCCI).

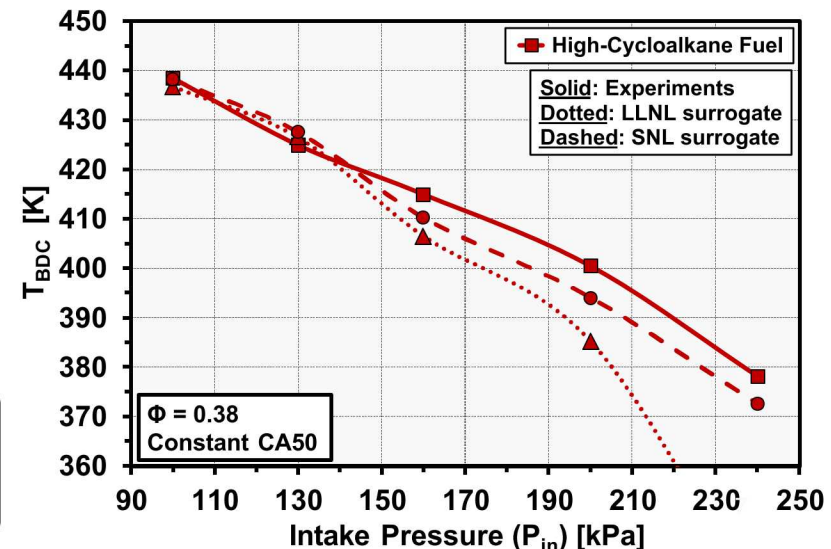
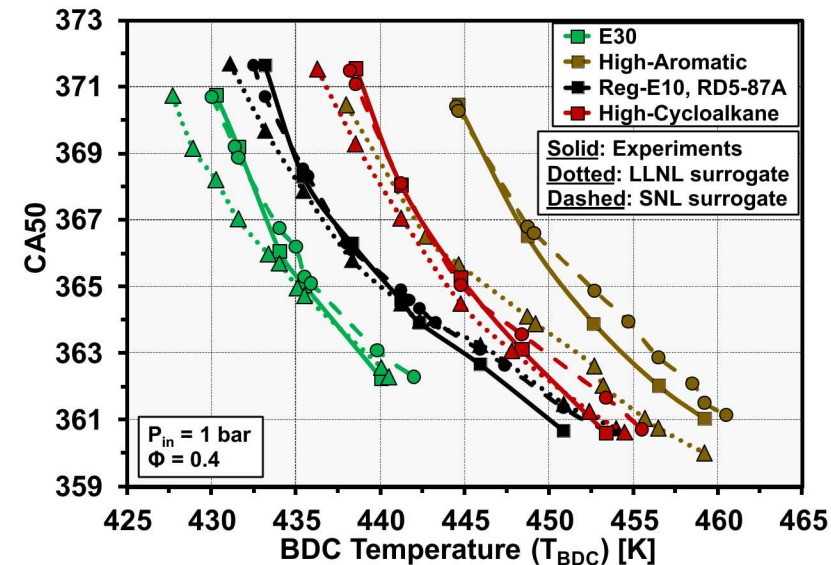
Required T_{in} or T_{BDC} Indicates Reactivity





- All modeling of engine combustion requires accurate kinetic mechanisms combined with appropriate surrogate blends for the fuel used.
 - Compare CHEMKIN results using LLNL detailed mechanism against fully premixed, well-characterized ACI (i.e. HCCI) expr. data.
 - $P_{in} = 1.0$ bar: Existing LLNL surrogates match trends, but w/ some significant discrepancies.
 - Developed new surrogates w/ 7-9 components that better match fuel composition from the detailed hydrocarbon analysis (DHA).
 - ⇒ **Improved match to experiment, all fuels.**
 - Also examined reactivity increase with boost:
 - High-cycloalkane example shows that existing surrogate gives large error at high boost.
 - The new surrogate, based on DHA, provides a much closer match with experimental data.
- Developing surrogates by selecting component types and quantities to match the DHA significantly improves results.

Required T_{BDC} Indicates Reactivity

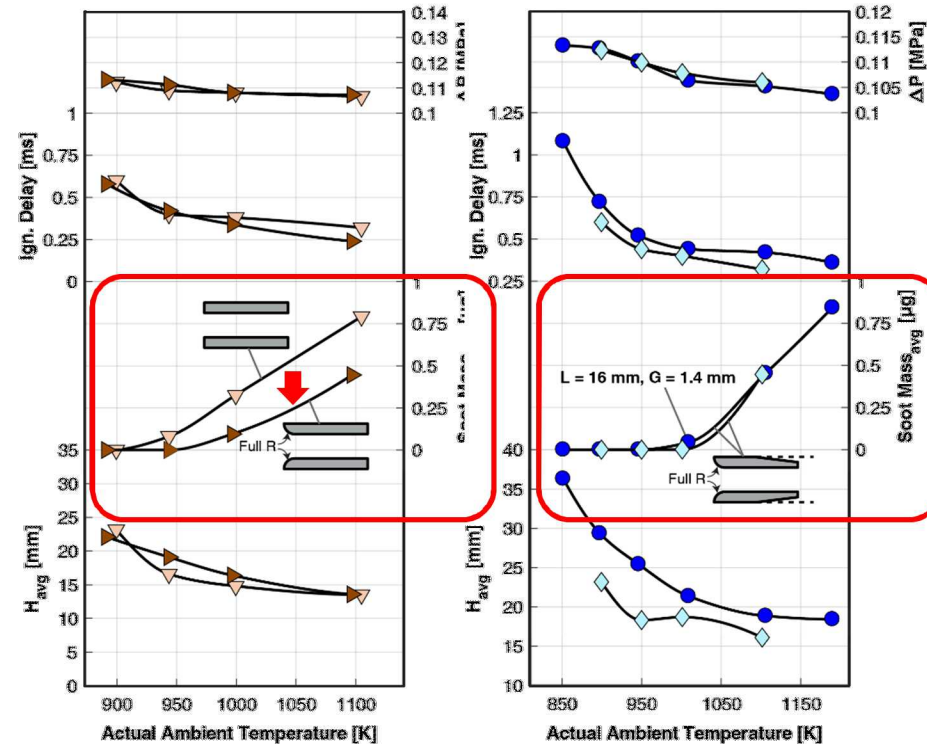
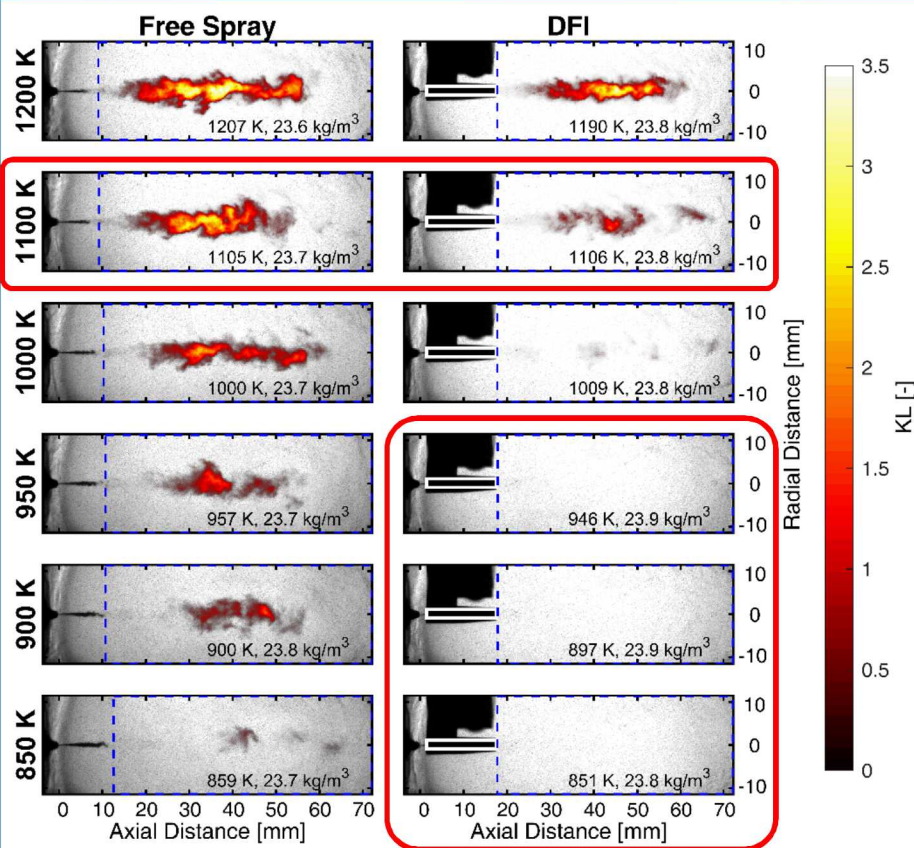




- DFI can attenuate soot levels in mixing-controlled CI spray flames by 35% to 100%
 - Soot quantified by diffused back illumination diagnostic

- Soot decrease can be improved by rounding the duct inlet
- Duct length can be shortened by 50% without adversely affecting performance
 - Facilitates installation in engines

Duct diam. = 2 mm, leng. (L) = 8 mm, gap (G) = 3.8 mm except where indicated

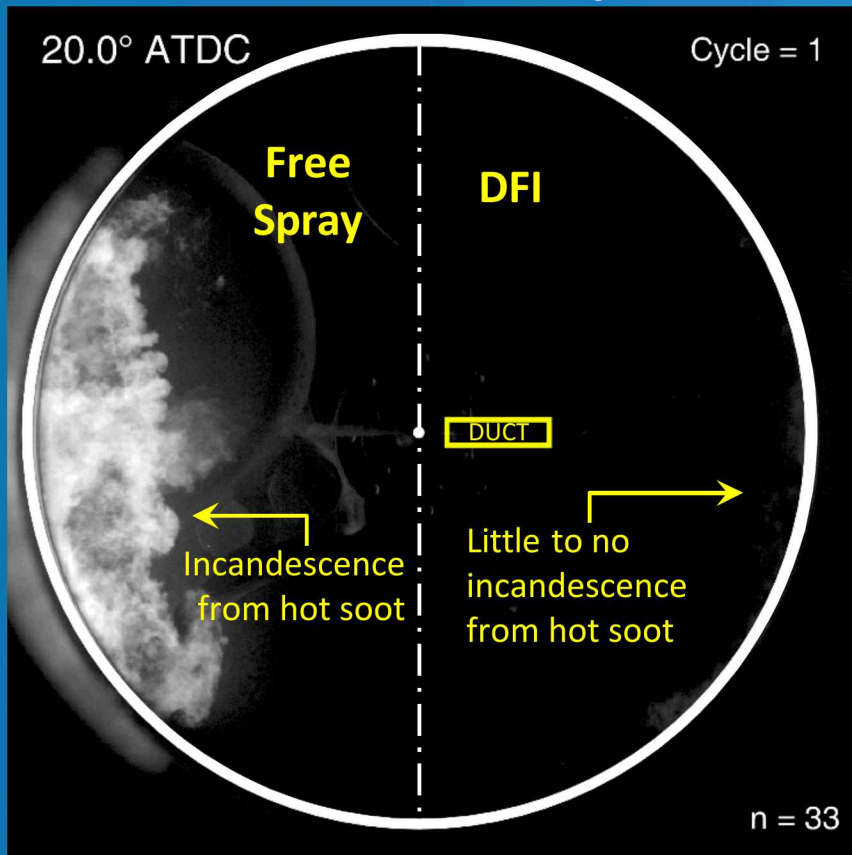


KL = soot absorbance; R = radius; H = flame liftoff length; ΔP = vessel pressure increase during combustion



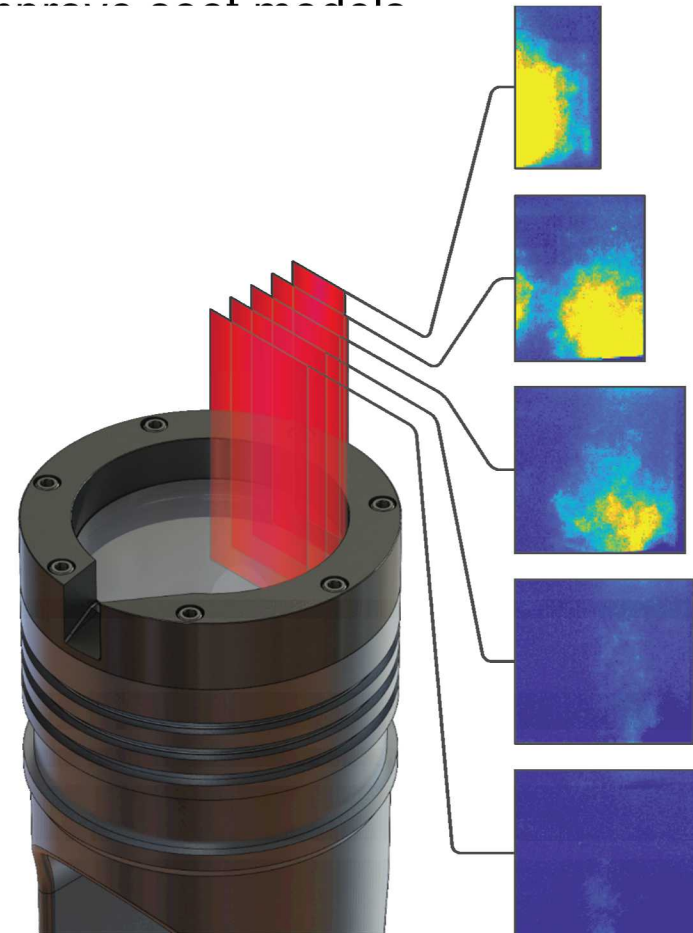
- Successfully conducted 1st testing of DFI in the optical engine
 - Using a two-hole injector tip and one duct

Natural Luminosity



ATDC = after top-dead-center; n = # of image in sequence

- Made in-cylinder soot volume-fraction field measurements using enhanced vertical laser-induced incandescence diagnostic
 - To improve soot models
 - To quantify soot emissions on scale
 - Collected data using a Laser Light Sheet (LLS)

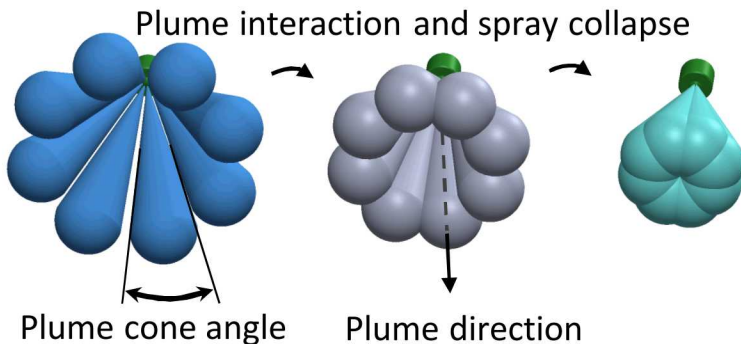
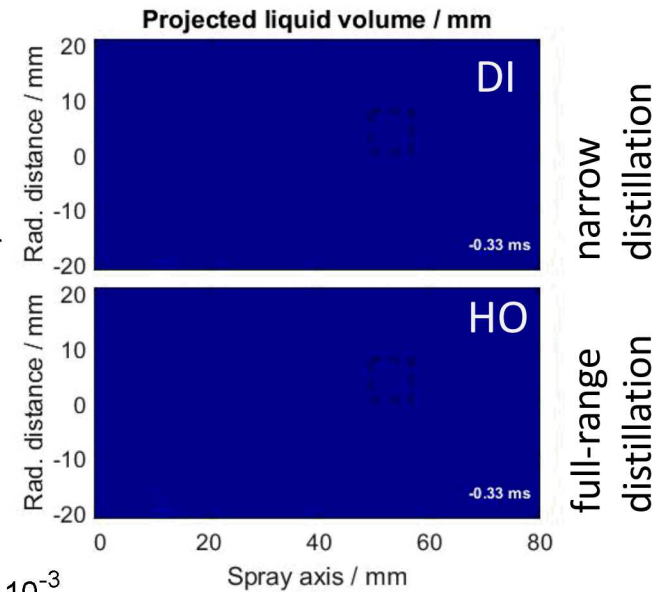


Spray Pattern Significantly Altered, Comparing Different Tier 3, RON-98 Fuels

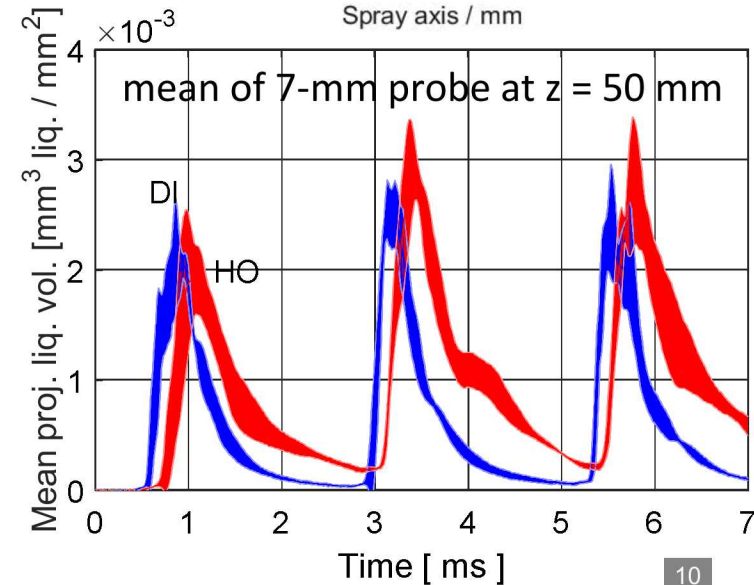


- Fuels tested in large constant-volume chamber:
 - DI: 20% di-isobutylene in surrogate BOB (blendstock for oxygenate blending)
 - HO: high-olefin BOB
- Liquid extinction imaging shows
 - Faster penetration for DI than HO
 - Substantial liquid penetration
 - DI has much faster and longer liquid penetration compared to high-olefin blend
 - But HO liquid persists after end of injection
- Significance
 - Light-component fuels can alter plume cone angle, affecting the entire fuel spray delivery

8-hole, 60° injector
 $T_{inj} = 90^\circ \text{ C}$
 $P_{inj} = 120 \text{ bar}$
 $t_{inj} = 0.6 \text{ ms}$
 $P_{gas} = 1 \text{ bar}$
 $T_{gas} = 170^\circ \text{ C}$



Collaboration with
M. Sjöberg and D.
Vuilleumier, with
experimental
assistance of E.
Cenker and S. Skeen



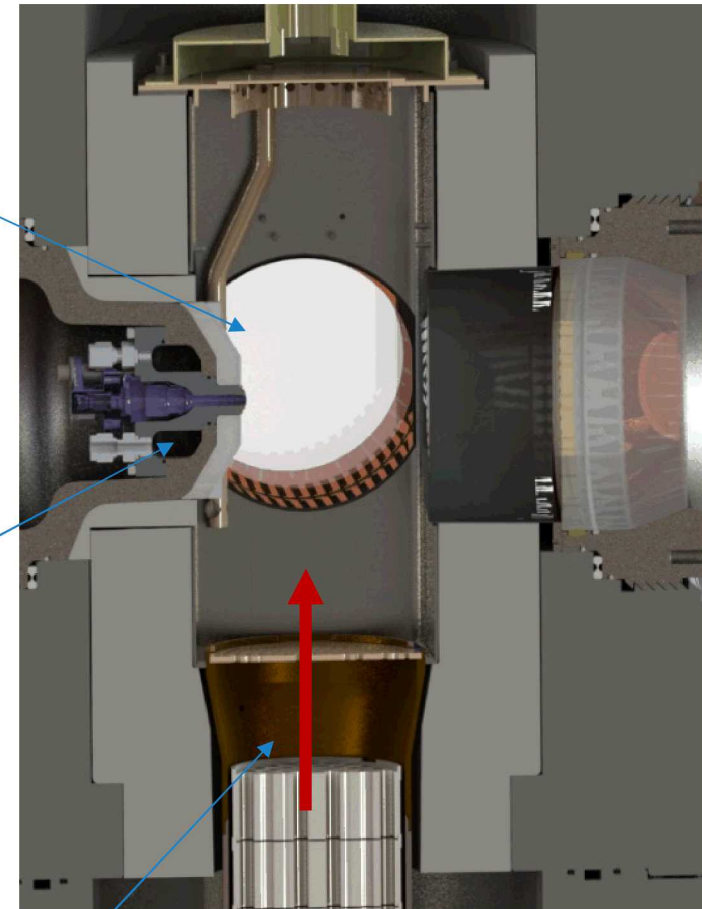


- Chamber capabilities
 - Large (125 mm) uniform temperature field with full optical access
 - Injection system flexibility for gasoline, diesel, or multimode
 - Small-volume fuel system (50 mL)
 - Mimics charge-gas conditions, even autoignition conditions for gasoline
 - Continuous scavenging results in massive increase in data throughput compared to constant-volume system
- Lab startup activities
 - All components complete
 - Final assembly in progress

Spray Chamber

Thermally
isolated
optically
accessible
spray test
section

Temperature
controlled
injector
jacket

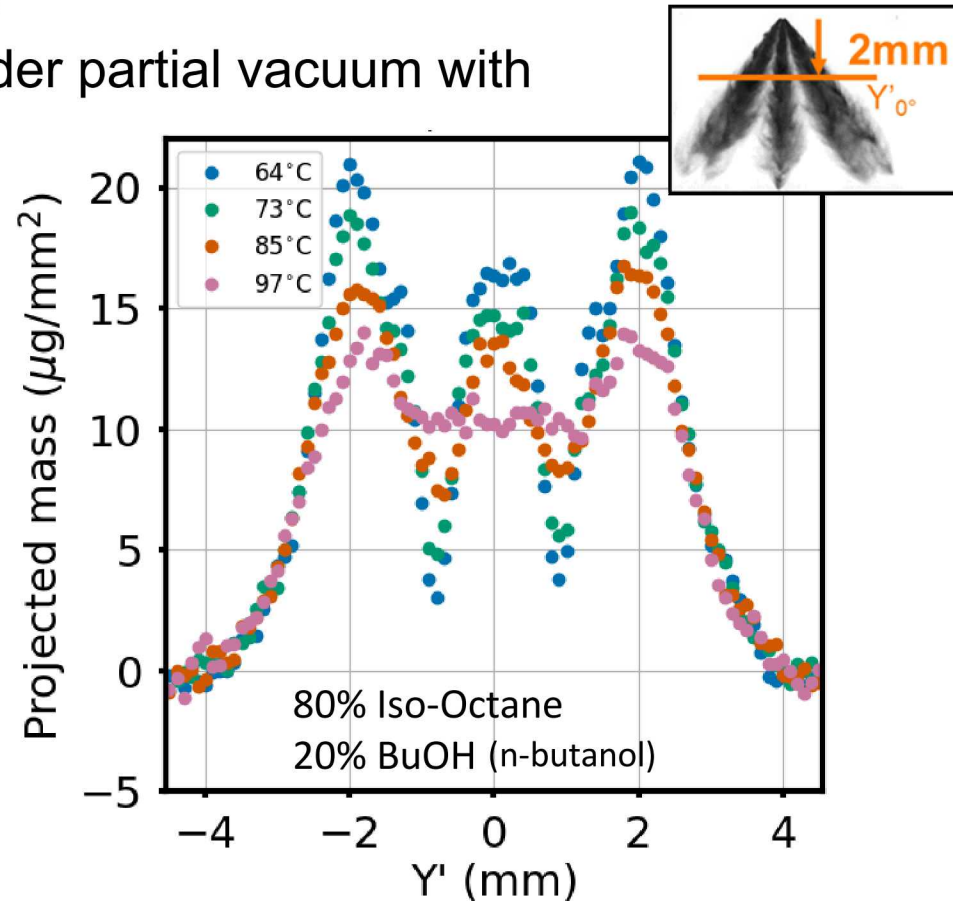


Heated air flow
up to 1100 K
vacuum to 150 bar

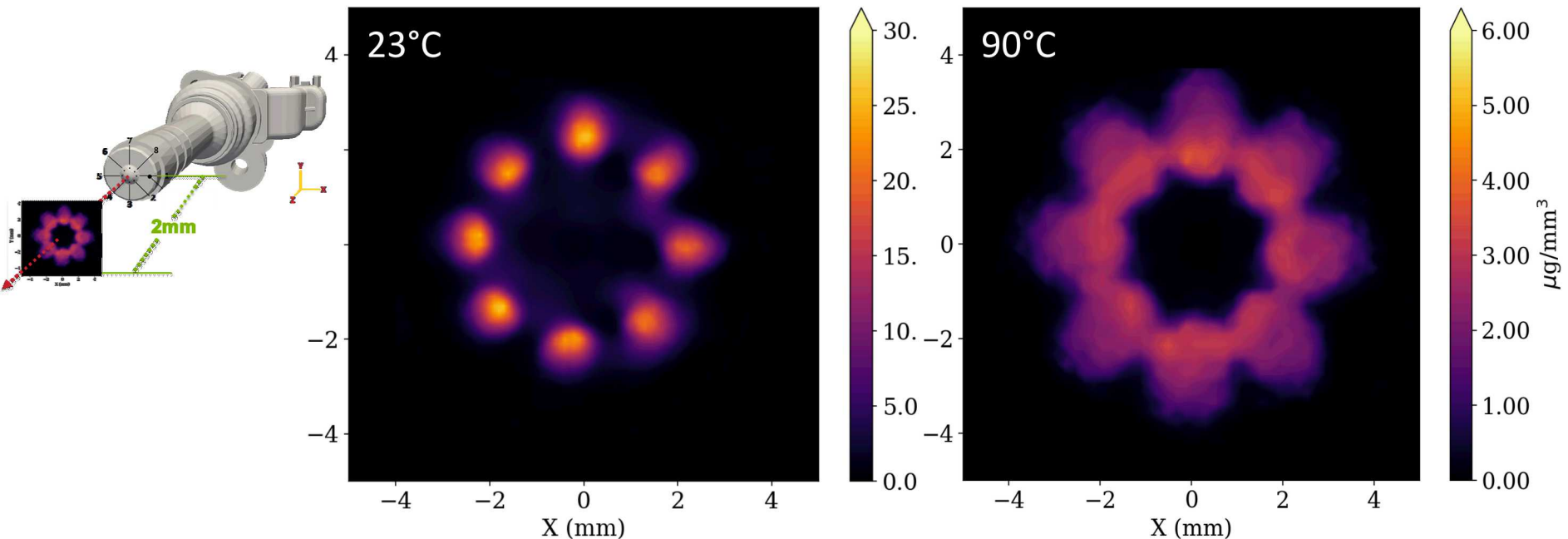
Temperature Sweeps Quantify the Onset of Flash-Boiling in GDI Sprays



- First measurements of the fuel mass distribution in the near-nozzle region of evaporating sprays
- New capability to measure fuels under partial vacuum with fuel temperature up to 100 °C
 - Simulates low-load, throttled GDI
- Measurements for 3 fuel blends
 - Iso-octane
 - Iso-octane with 20% ethanol
 - Iso-octane with 20% butanol
- Measurements were made spanning a range of fuel temperatures
 - To quantify the change in the fuel distribution during the transition to flash-boiling
- As temperature increases, fuel evaporates more readily, plumes become less distinct



A slice through the fuel mass distribution 2 mm from the nozzle at 4 fuel temperatures



2D slices obtained using x-ray tomography showing the iso-octane density under room temperature and flash-boiling conditions

- Liquid fuel density has been quantified only 2 mm downstream of the injector for three different fuel blends
- As expected, spray plumes are more diffuse under flash-boiling cond's
- Measurement cond's nearly match ECN's "Spray G2" flash-boiling cond'n
- Simulations from several groups will be compared with the measurements at the ECN6 Workshop



- Implemented dynamic link to REFPROP library (by NIST¹)

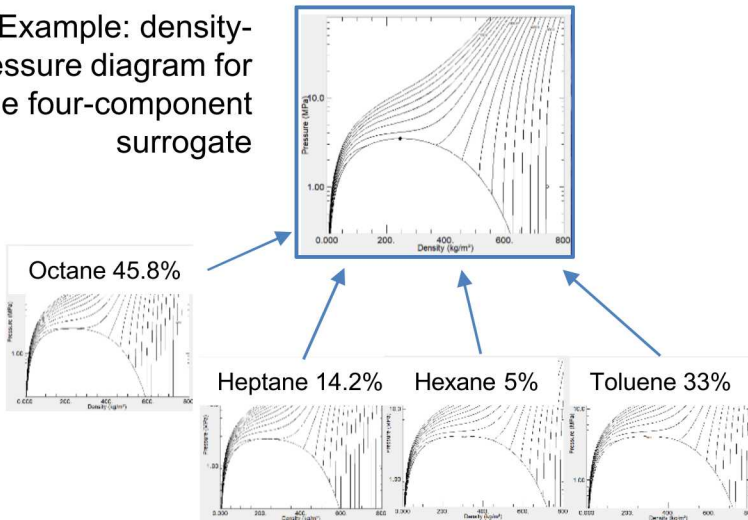
Mixture rules for Helmholtz energy are used to generate run-time accurate equation of state and heat of vaporization of the blendstock:

$$a = a^{\text{idsol}} + a^{\text{excess}}$$

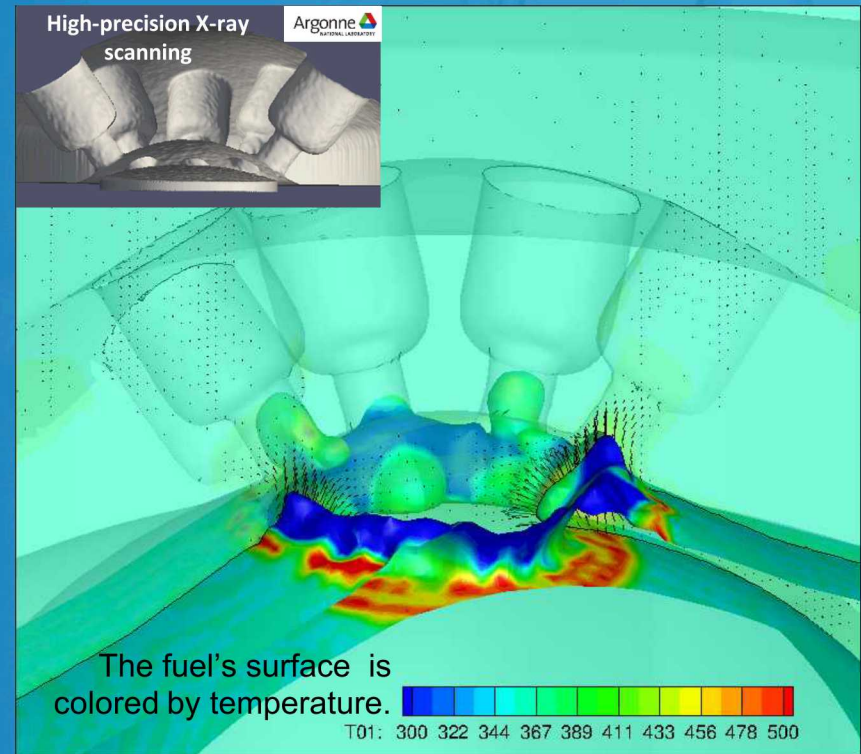
$$a^{\text{idsol}} = \sum_{j=1}^m x_j [a_i^0(\rho, T) + a_i^r(\delta, \tau) + RT \ln x_j]$$

$$a^{\text{excess}} = RT \sum_{i=1}^{m-1} \sum_{j=i+1}^m x_i x_j F_{ij} \sum_k N_k \delta_k^{d_i} \tau_k^{t_i} \exp(-\delta^{l_k})$$

Example: density-pressure diagram for the four-component surrogate



- GDI ongoing simulation with multiphase CLSMOF code and REFPROP library



The fuel's surface is colored by temperature. T01: 300 322 344 367 389 411 433 456 478 500

Snapshot of partially-filled Spray G chamber during start of injection. The fuel has the thermophysical properties of the NREL² four-component BOB.

¹NIST = National Institute for Standards and Technology; ²NREL = National Renewable Energy Laboratory

Responses to Previous Year's Reviewers' Comments



<p>All</p>	<p>P. 5-74: The “presentation & slides are extremely confusing & difficult to follow”; “slides introduce many unfamiliar acronyms without defining or explaining them.”</p> <ul style="list-style-type: none"> <i>We changed to a color-coded tabular format this year in attempt to minimize confusion, as well as trying to simplify messages. All uncommon acronyms are defined at first use.</i>
<p>ACI-F</p>	<p>Page 5-73: Reviewer questioned using low-temperature gasoline combustion (LTGC) & relevance to multi-mode HCCI/boosted-SI engines.</p> <ul style="list-style-type: none"> <i>HCCI is a subset of LTGC, and fuels testing is conducted at well-mixed HCCI conditions with temps. and pressures relevant to ACI, including multi-mode engines using HCCI at low loads.</i>
<p>MCCI</p>	<p>P. 5-73: The “ducted combustion concept is interesting, but does not seem to fit well in the Co-Optima structure...perhaps continue it as a separate project.”</p> <ul style="list-style-type: none"> <i>We have made proposals to cover DFI research that is not related to fuel effects using other funding sources, and believe that this might occur in FY19.</i>
<p>SCO</p>	<p>Page 5-77: “Fuel sprays have a major effect on emissions...encouraging that DoE has allocated some of its most sophisticated spray measurement equipment to this task.”</p> <ul style="list-style-type: none"> <i>The support is appreciated particularly because this project has made a substantial investment into a chamber for higher quality spray diagnostics for the future.</i>
<p>SX</p>	<p>Page 5-76: “Some work apparently was delayed...such as X-ray studies of baseline fuel under flash[ing] & non-flashing conditions in the new high-press. fuel system”</p> <ul style="list-style-type: none"> <i>There were delays in fuel system procurement & equipment failures trying to reach flash-boiling cond's. These have been overcome, & all 2018 milestones are complete/on-track.</i>
<p>SS</p>	<p>No reviewer comments; this project was a new start in FY18.</p>

Collaboration and Coordination with Other Institutions



ACI-F	<ul style="list-style-type: none">• LLNL (Pitz) : Validation of kinetic mech's & discussions on formulating surrogates• LLNL (McNenly): Searches for Co-Optima fuels with potential phi-sensitivity• ANL (Goldsborough): Comparison of RCM¹ autoign. data with Sandia engine data• ORNL² (Szybist): Computations corroborate Sandia expr. data on fuel reactivities
MCCI	<ul style="list-style-type: none">• Caterpillar, Ford, and Georgia Tech: DFI CRADA³• Coordinating Research Council: diesel surrogate fuel development & testing• High-Performance Fuels Team (Co-Optima): fuel candidates for MCCI applications• Caterpillar & McNenly (LLNL): quantitative in-cylinder soot diagnostic
SCO	<ul style="list-style-type: none">• ECN: data are being shared, several modeling groups are expected to contribute simulations for comparison with the measurements
SX	<ul style="list-style-type: none">• Sandia: coordination with Pickett on measurement conditions• ECN: data are being shared, several modeling groups are expected to contribute simulations for comparison with the measurements
SS	<ul style="list-style-type: none">• Prof. Mark Sussman, Florida State Univ.: Development & testing of numerical methods for fuel injection applications• Center for Computational Sciences & Engineering, Berkeley Lab: Development of library for hierarchical adaptive mesh refinement in high-performance computing

¹RCM = rapid compression machine; ²ORNL = Oak Ridge National Lab.; ³CRADA = cooperative research and development agreement

Remaining Challenges and Barriers



ACI-F	<ul style="list-style-type: none">• Develop & test fuels containing HPF¹ blendstocks selected to improve ACI-engine performance vs. the Co-Op core fuels that were designed primarily for boosted SI.• A greater understanding is required of how a fuel's Φ-sensitivity and ITHR² is related to its molecular structure to facilitate selection of HPF blendstocks for ACI.
MCCI	<ul style="list-style-type: none">• Unknown sensitivities of DFI-engine efficiencies (comb. & thermal) & regulated emissions to changes in basic parameters: e.g., engine operating conditions, fuel-injection parameters, duct geometric characteristics, and fuel properties.• Level of composition/property accuracy req'd for diesel surrogate fuels is unclear.
SCO	<ul style="list-style-type: none">• Liquid wall impingement is difficult to characterize but is closely linked to soot and PM³ emissions. Tailoring fuel delivery for multimode ignition/combustion requires precise control to maintain controlled flame while not forming PM.
SX	<ul style="list-style-type: none">• Current measurements using x-ray radiography cannot distinguish between liquid fuel and fuel vapor. X-ray fluorescence measurements are more challenging, but will allow us to quantify the liquid and vapor separately.
SS	<ul style="list-style-type: none">• A major barrier is the high computational cost of a detailed fuel injection simulation, which limits how many operation points can be examined. The development of a data-driven process capable of integrating spray details in combustion simulations at the engine scale remains a substantial challenge.

¹HPF = Co-Optima High-Performance Fuels Team; ²ITHR = intermediate-temperature heat release; ³PM = particulate matter

Proposed Future Research



ACI-F	<ul style="list-style-type: none">• Develop and test fuels containing HPF blendstocks selected to improve their ACI-engine performance.• Test the new surrogate blends in the engine to verify their performance and to guide development of further surrogate improvements.
MCCI	<ul style="list-style-type: none">• Conduct optical-engine experiments to assess diesel surrogate fuels.• Determine effects of Co-Optima blendstocks on DFI via optical-engine tests.• Quantify sensitivity of DFI to changes in engine oper. cond's & duct config.• Increase DFI-engine load capability via fuel and/or configuration changes.
SCO	<ul style="list-style-type: none">• Quantify liquid penetration, plume direction and plume shape.• Measure soot concentration with and without forced ignition for range of gasoline and diesel fuels.• Perform stratified-ignition experiments at relevant T and P.
SX	<ul style="list-style-type: none">• X-ray imaging of cavitation in steel diesel injection nozzles.• Add'l measurements of flash-boiling GDI sprays using x-ray fluorescence.
SS	<ul style="list-style-type: none">• Analyze effects of differential evaporation, which results from the different heat-of-vaporization properties of different surrogate-fuel components.• Implement more-detailed computational models for cavitation and flash-boiling, in relation to the operation mode of modern injectors.

Summary



ACI-F	<ul style="list-style-type: none">• Showed that even when RON & MON are held constant, fuel composition has a large effect on ACI autoignition reactivity. RON/MON are not sufficient.• Discovered that the high-cycloalkane fuel has the least reactivity increase with boost, indicating that it should be very good for boosted-SI engines.• Developed new fuel surrogates that closely match experimental data.
MCCI	<ul style="list-style-type: none">• Showed that DFI lowers soot, not just soot luminosity.• Discovered DFI configuration changes to facilitate packaging in an engine.• Implemented hardware to successfully test DFI in the optical engine.• Developing a quantitative in-cylinder soot diagnostic to measure fuel effects.
SCO	<ul style="list-style-type: none">• Showed major variation in spray mixing for leading-candidate fuels.• Chamber developed offering significant diagnostic advancements.
SX	<ul style="list-style-type: none">• Near-nozzle fuel distributions have been measured for three fuel blends, several fuel temperatures, and for the first time, under vaporizing and non-vaporizing conditions. The results have been shared with modeling groups for development and validation of vaporizing spray simulations.
SS	<ul style="list-style-type: none">• The NIST thermodynamic and transport properties database is now accessed by the Sandia research code CLSMOF in the multiphase CFD simulation of fuel injection. This new capability is demonstrated for NREL's 4-component BOB in an ongoing GDI simulation.



Technical Back-Up Slides

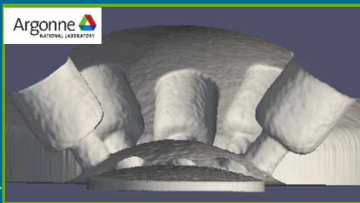
Computational Approach: The Multiphase Code CLSMOF



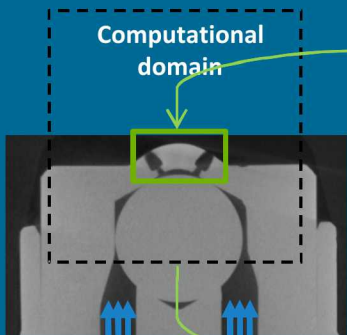
- Sharp-interface discretization of multi-phase Navier-Stokes eqns.
 - ✓ Compressible effects
 - ✓ Adaptive mesh refinement
 - ✓ Non-conformal, moving wall boundaries
 - ✓ Flexible equation of state implementation

ECN Spray G (8-hole GDI)

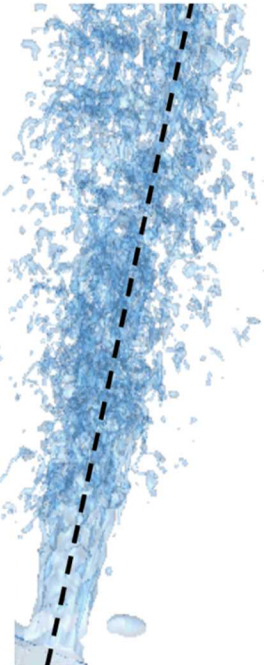
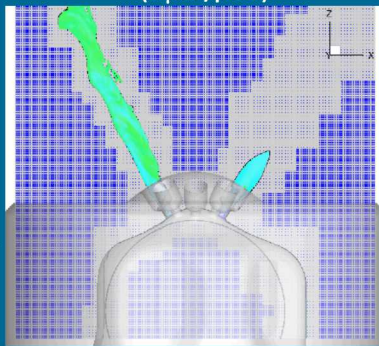
Injector surfaces are reconstructed from X-ray radiography and converted into a computational mesh



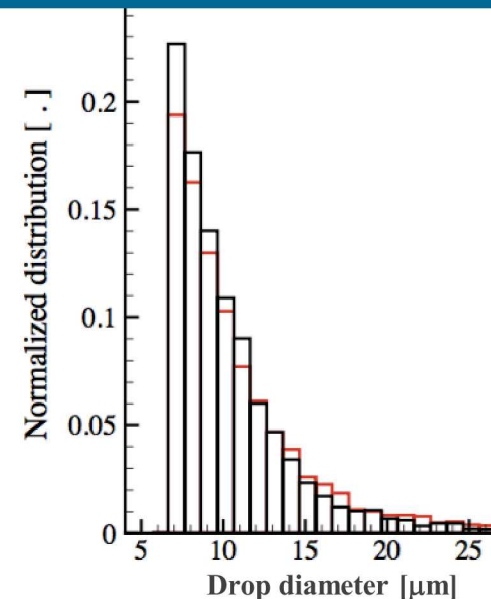
High-precision scanning
(1 μm / pixel)



CLSMOF ongoing simulation with embedded boundary



Spray statistics



Increased scalability up to 900M cells (10,000 MPI processes on SNL and ANL platforms) with hybrid MPI / Open MP configuration.



Reviewer-Only Slides

Publications and Presentations



ACI-F	<p>Presentations</p> <ol style="list-style-type: none"> 1. Dec, J.E., Ji, C., Dernette, J., and Gentz, G., “Boosted-SI” Fuel Compatibility with LTGC and the Use of RON & MON as Autoignition Metrics,” Co-Optima Stakeholder Meeting, August 2017. 2. Dec, J.E., Gentz, G., and Lopez-Pintor, D., “Performance of the High-Cycloalkane RON98 Fuel,” GM/Sandia Working Group Meeting, February 2018. 3. Dec, J.E. and Pitz, W.J., “Medium/Heavy-Duty Kinetically Controlled ACI,” Co-Optima All Hands Meeting, March 21-22, 2018. 4. Lopez-Pintor, D. and Dec, J.E., “Φ-Sensitivity for LTGC / ACI Engines: Understanding the Fundamentals & Tailoring Fuel Blends to Maximize this Property,” Co-Optima All Hands Meeting, April 18, 2018.
MCCI	<p>Publications</p> <ol style="list-style-type: none"> 1. Gehmlich, R.K., Mueller, C.J., Ruth, D.J., Nilsen, C.W., Skeen, S.A., and Manin, J., “Using Ducted Fuel Injection to Attenuate or Prevent Soot Formation in Mixing-Controlled Combustion Strategies for Engine Applications,” submitted to <i>Applied Energy</i>, Jan. 18, 2018. 2. Yasutomi, K., Mueller, C.J., Pickett, L.M., and Skeen, S.A., “Investigation of the spray and combustion characteristics of four multi-component diesel surrogate fuels relative to their commercial target fuel,” accepted to <i>THIESEL 2018 Conference on Thermo- and Fluid Dynamic Processes in Direct Injection Engines</i>, Valencia, Spain, Sept. 11-14, 2018. 3. Mueller, C.J. and Gehmlich, R.K., “Mixing-Controlled Combustion in a Heavy-Duty Compression-Ignition Engine,” in <i>The Gallery of Combustion and Fire</i>, Ed. by C. Baukal, Cambridge Univ. Press, <i>in press</i> 2018. 4. Mueller, C.J., Nilsen, C.W., Ruth, D.J., Gehmlich, R.K., Pickett, L.M., and Skeen, S.A., “Ducted Fuel Injection: A New Approach for Lowering Soot Emissions from Direct-Injection Engines,” <i>Applied Energy</i> 204:206-220, 2017, doi:10.1016/j.apenergy.2017.07.001. <p>Presentations: 15 from this project since last 2017 DOE Annual Merit Review meeting, 1 invited.</p>
SCO	<ul style="list-style-type: none"> • None
SX	<ul style="list-style-type: none"> • None
SS	<ul style="list-style-type: none"> • None

Critical Assumptions and Issues



ACI-F	<ul style="list-style-type: none">• None.
MCCI	<ul style="list-style-type: none">• So little is known about DFI that it is difficult to evaluate its potential as an ultimately production-viable engine technology.
SCO	<ul style="list-style-type: none">• While variation in spray mixing is reported for different Tier-3 fuels, there really has not been an attempt to change the injector to match a specific fuel to date. Presumably, the spray could be altered for a given fuel injector design and schedule to provide additional benefits to the engine.
SX	<ul style="list-style-type: none">• The current data analysis procedures assume that x-ray absorption is solely due to liquid fuel. However, the fuel vapor contributes a small amount to the signal, and the vapor displaces the ambient gas, changing the background signal. These factors increase the error bars in the current measurements. Future measurements using X-ray fluorescence will allow us to quantify the liquid, vapor, and ambient gas independently.
SS	<ul style="list-style-type: none">• The in-cylinder flow conditions are such that the fuel can be considered sub-critical up to its evaporation.