SAND2018-12700R

Advanced Light-Duty SI Engine Fuels Research

Magnus Sjöberg, Principal Investigator
David Vuilleumier, Namho Kim
Organization: Sandia National Laboratories
Address: MS9053, PO Box 969
Livermore, CA 94551-0969
Phone: (925) 294-3635
E-mail: mgsjobe@sandia.gov

Kevin Stork, DOE Program Manager
U.S. Department of Energy
Phone: (202) 586-8306
E-mail: Kevin.Stork@ee.doe.gov

Start Date: 10/01/2017 End Date: 9/30/2018
Project Funding: $708,000 DOE share: $708,000 Non-DOE share: $0

Project Introduction

This project furthers the science-base needed by industry stakeholder to co-evolve the next generations of highly efficient DISI engines and new gasoline-type fuels. Here, the research emphasis is on lean operation, which can provide high efficiency, using fuels that also support traditional non-dilute stoichiometric operation for peak load and power. Lean operation induces challenges with ignition stability, slow flame propagation and low combustion efficiency. Therefore, techniques that can overcome these challenges are studied. Specifically, fuel stratification is used to ensure ignition and completeness of combustion, but this technique has soot- and NO_x- emissions challenges. For ultra-lean well-mixed operation, turbulent deflagration can be combined with controlled end-gas autoignition to render mixed-mode combustion for sufficiently fast heat release. However, such mixed-mode combustion requires appropriate autoignition reactivity, motivating fuel studies of autoignition under lean conditions.

Objectives

- Provide the science-base needed to understand how emerging alternative fuels impact highly efficient DISI light-duty engines being developed by industry.
- Elucidate how engine design and operation can be optimized for clean and efficient use of future fuels.
- Develop and apply advanced optical diagnostics for probing in-cylinder processes.

Approach

The Alternative Fuels DISI Engine Lab at Sandia houses an engine that is capable of both performance testing and in-cylinder optical diagnostics. First, performance testing with an all-metal engine configuration is conducted over wide ranges of operating conditions and alternative fuel blends. This allows quantifying fuel-efficiency and exhaust emissions behavior. Second, in-cylinder processes are examined with high-speed optical diagnostics, including advanced laser-based techniques. This reveals the mechanisms that govern the combustion process and exhaust-emissions formation. Computer modeling provides additional insight of the governing combustion fundamentals. The combination of performance testing, exhaust-emissions measurements, optical diagnostics, and modeling allows building a comprehensive science-base.

Results

Key accomplishments for Fiscal Year 2018 :

- Assessed the relevance of PMI for nine fuels across three stoichiometric well-mixed and two lean stratified operating conditions.
- Developed in-cylinder soot diagnostics based on diffuse back illumination (DBI), and used it to quantify in-cylinder soot mass distributions for key operating points.

- Used wall-wetting diagnostics based on refractive index matching (RIM) to determine the role of fuel films for in-cylinder soot production.
- Showed that high smoke emissions for cold-start stratified-charge operation with an E30 fuel can be traced to increased fuel films on the piston top, with associated sooting pool fires.
- Acquired lean mixed-mode combustion data for five fuels, spanning a range of ϕ, P_{in}, T_{in} and $[O_2]$ conditions.
- Performed an initial assessment of the efficacy of Octane-Index framework for lean conditions.

In the following sections, selected examples of the FY2018 accomplishments are presented.

Fully Stratified Operation – Spray-guided, stratified-charge SI operation can provide high thermal efficiency for low and mid loads, where a light-duty automotive engine typically spends a large fraction of time. However, while enabling high-efficiency operation, fuel stratification can cause unacceptably high engine-out smoke levels, depending both on the fuel injection and combustion strategy, and the fuel composition. A commonly used metric for a fuel's sooting propensity is the Particulate Matter Index (PMI), which originally was developed for port fuel injection (PFI) engines [Aikawa *et al.*]. In the current effort, the efficacy of PMI is assessed for a direct injection (DI) engine, operating in either stratified-lean or well-mixed stoichiometric mode. This work includes the use of fuel components that were not emphasized during the original development of the PMI metric, such as various alcohols. For brevity, only results for stratified operation are presented in this report. For stratified naturally aspirated operation at 1,000 rpm, the light-blue squares in Fig. 1 show that for most fuels, the measured engine-out soot (as derived from paper darkening in an AVL 415S Smoke Meter) scales relatively well with PMI. However, the two ethanol-containing fuels E30 and RD5-87 (E10) fall well above the dashed linear trend line, which was based on the seven non-ethanol fuels (shown connected by solid lines). In-cylinder optical diagnostics reveal that under these conditions, the E30 fuel impinges on the piston top, causing wall-wetting and associated pool fires, as discussed in [Ding *et al.*, and He *et al.*]. The elevated smoke emissions with E30 become even more severe for operation with a reduced coolant temperature, such as during warm-up, as shown in the top row of Fig. 2. The imaging presented in this figure shows that the liquid fuel films become thicker and larger with a reduction of the coolant temperature. As a result, the combustion becomes more strongly sooting, explaining the increased smoke emissions.

Furthermore, Fig. 1 shows that when the operating conditions change to a higher-speed, boosted condition, represented by brown circles, the effect of ethanol reverses. Here, the E30 fuel falls well below the dashed linear trend line. At this slightly boosted operating point, optical diagnostics reveal that both the wall wetting and pool-fire activity are strongly reduced for all fuels. As a result, it is hypothesized that the soot-formation pathway becomes dominated by bulk-gas soot processes, partly augmented by a tumble-induced fuel-vapor asymmetry [Zeng *et al.*]. In this situation, the fuel-borne oxygen of the ethanol in the E30 fuel helps to suppress soot formation. It should be noted that the calculation of PMI does not take the oxygen content of the fuel into account.

For a better understanding of fuel effects on bulk-gas soot-formation processes, a new in-cylinder soot diagnostic was developed and used, as depicted in Fig. 3. Using diffuse back illumination (DBI), the amount of in-cylinder soot can be quantified on a crank-angle resolved basis. The initial results indicate strong fuel effects, and also substantial cycle-to-cycle variations. Figure 4 provides an example of a strongly sooting cycle for a fuel that contains diisobutylene (DIB), with elevated soot concentration on the intake side of the combustion chamber. Looking back at Fig. 1, it can be seen that the DIB blend falls well above the average trend line for operation at 2,000 rpm. In combination with direct flame imaging, the DBI diagnostics confirms that the DIB fuel produces elevated in-cylinder soot to a degree that is inconsistent with its low PMI.

Lean Autoignition Studies – Lean or dilute well-mixed SI engine operation can improve thermal efficiency, but a key challenge is to maintain a 10-90% burn duration shorter than 30°CA, which is needed to realize efficiency gains of lean combustion [Ayala and Heywood]. Lean deflagration has a tendency to cause a slow burn-out process, but a speed-up can achieved via the use of mixed-mode combustion, which features a combination of turbulent deflagration and end-gas autoignition [Sjöberg and Zeng, 2016]. Practical implementation of mixed-mode combustion (or other advanced compression ignition strategies) requires that suitable fuels are available in the marketplace, and that appropriate autoignition metrics are available to specify the fuels being used. Consequently, the applicability of RON and MON for autoignition under lean conditions is currently being assessed for a range of fuels. For these experiments, several injections during the intake stroke create a well-mixed fuel-air charge. However, to stabilize flame development for these lean conditions, a small amount of extra fuel (1.6mg ≈ 10% of the total fuel mass) is injected at the time of spark to enrich the mixture near the spark plug. This injection strategy is called partial fuel stratification (PFS).

Figure 5 shows a comparison of lean autoignition reactivity for five fuels over a range of intake oxygen mole fractions [O_2]. The autoignition metric used here is based on a determination of the combustion phasing (CA50) where the amount of end-gas autoignition is marginal, as outlined in [Sjöberg *et al.* 2017]. It can be observed that the autoignition reactivity varies substantially between fuels, with the RON91 fuel being the most reactive, therefore requiring a less advanced combustion phasing for the beneficial end-gas autoignition to take place. These well-controlled tests utilize electric intake air heating to promote autoignition. In a practical implementation, elevated charge temperature can be achieved by retaining hot residual gases, which would lower [O_2] of the reactants. Figure 5 shows that the response to changes of the intake [O_2] varies between fuels, with the High Cycloalkane fuel being the least sensitive. The differences in [O_2] sensitivity could have consequences for a practical engine implementation that uses retained residuals or exhaust-gas recirculation (EGR).

Figure 6 provides an example of the ability of the Octane Index to rank order the fuels' autoignition reactivity. The best-fit K-factor is 0.51 for operation with [O_2] = 15.5%, notionally placing the autoignition regime right in between the RON (K=0) and the MON (K=1) tests. The quality of the fit is good over this selection of fuels, with an R^2 value of 0.92. Future work will expand the assessment of the octane index to other conditions, and will include fuels that contain alcohols and other classes of molecules.

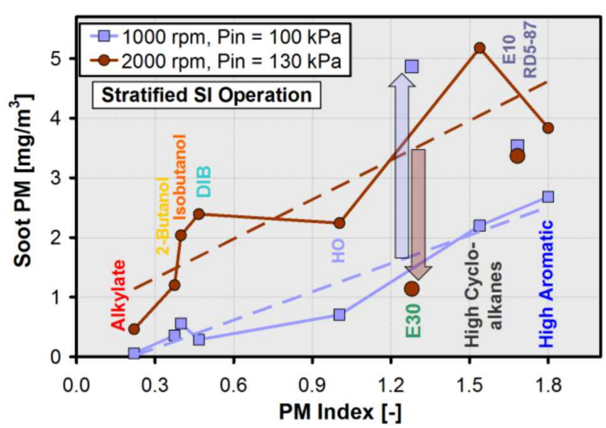

Figure 1. For naturally aspirated stratified-charge, direct-injection SI operation at 1,000 rpm, smoke emissions for E30 are much higher than the average trend line due to the formation of pool fires. For boosted operation at 2000 rpm, E30 suppresses soot formation. Intake [O_2] = 17%, ϕ_m = 0.33, $T_{coolant}$ = 75°C. PMI values were provided by [Fouts et al., 2018] and [Christensen, et al. 2018]. Figure by Magnus Sjöberg, SNL.

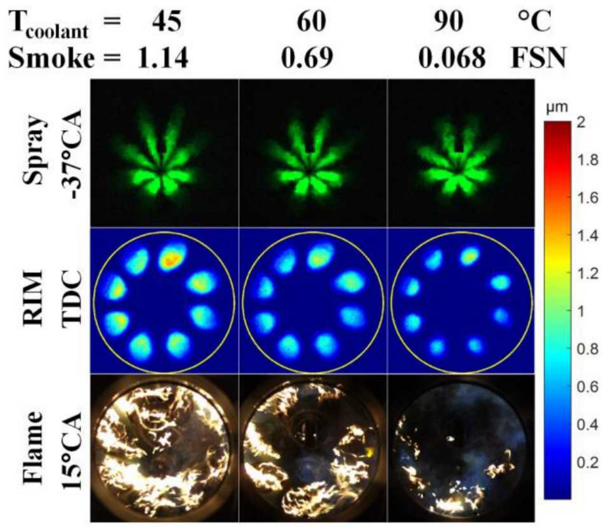

Figure 2. Effect of engine coolant temperature on piston-top wall wetting and associated formation of sooting pool-fires and exhaust smoke emissions. Intake [O_2] = 18%. Figure by Magnus Sjöberg, SNL, and Xu He, BIT.

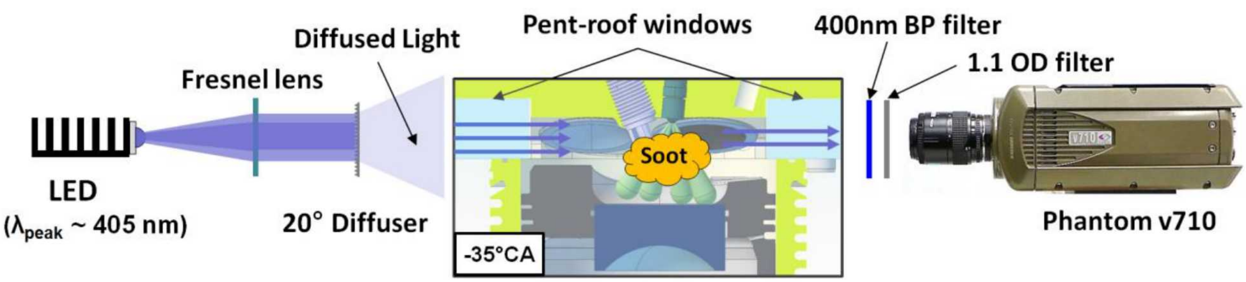

Figure 3. Schematic of diffuse back illumination (DBI) setup for in-cylinder soot quantification. Figure by Namho Kim, SNL.

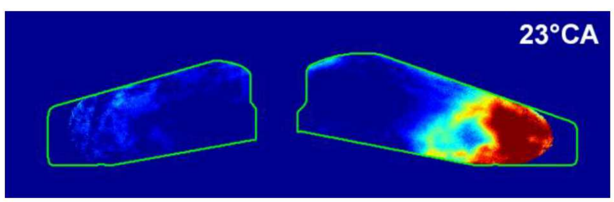

Figure 4. Detection of in-cylinder soot for stratified operation with a RON98 fuel containing 19.6% diisobutylene (DIB) by volume. Figure by Namho Kim, SNL.

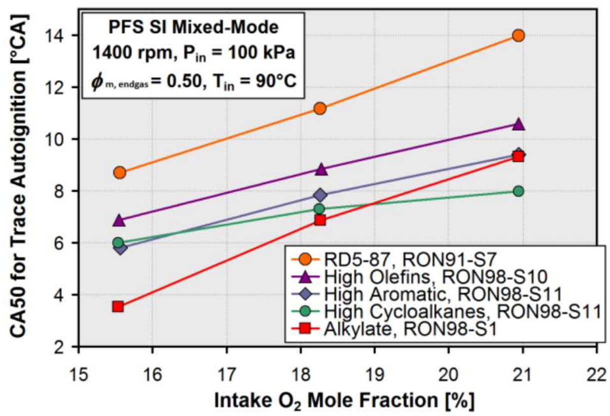

Figure 5. Effect of intake oxygen mole fraction on combustion phasing rendering "trace autoignition" for lean SI operation with ϕ_m = 0.50 in the end-gas. Figure by Magnus Sjöberg, SNL.

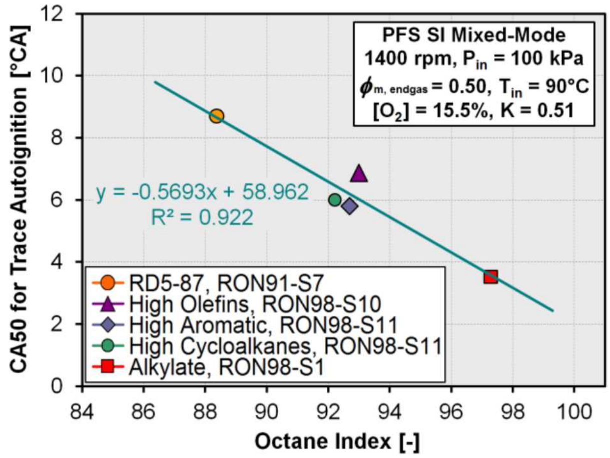

Figure 6. Example of the application of the octane-index framework for lean mixed-mode combustion utilizing end-gas autoignition. P_{in} = 100 kPa. Figure by Magnus Sjöberg, SNL.

Conclusions

These research tasks are contributing strongly to both the Co-Optima project and to the fundamental science of fuel/combustion interactions for advanced SI engine combustion.

For advanced lean stratified-charge operation, the smoke/soot emissions can be reasonably well correlated with the fuels' PMI values, but with some noteworthy exceptions. For conditions that are prone to wall wetting, the ethanol content of an E30 fuel can cause pool fires and smoke emissions that are strongly elevated relative to expectations based on PMI. In contrast, for boosted conditions dominated by bulk-gas soot formation, the oxygen content of the E30 fuel acts to suppress soot formation. Also, for these boosted conditions, a fuel containing diisobutylene shows higher than expected in-cylinder soot and exhaust smoke emissions. These findings with regards to wall wetting, pool fires, and bulk-gas soot formation highlight the need to further develop fuel-property metrics that can better predict the effect of fuel on engine PM emissions, even for advanced stratified-charge operation utilizing non-conventional gasoline-type fuels.

For lean mixed-mode combustion, fuels can exhibit different responses to changes of the intake oxygen mole fraction, implying differences in the response to retained residuals or EGR for a practical implementation. Using a small set of fuels, it was demonstrated that the Octane-Index framework can be applicable for rank ordering fuels in terms of their lean autoignition reactivities. However, both the fuels matrix and experimental matrix need to be expanded for future studies.

References

Aikawa, K., T. Sakurai, and J. Jetter, "Development of a Predictive Model for Gasoline Vehicle Particulate Matter Emissions," SAE Int. J. Fuels Lubr. 3(2):610-622, 2010, doi: 10.4271/2010-01-2115.

Ayala, F. and J. Heywood, "Lean SI Engines: The role of combustion variability in defining lean limits," SAE Technical Paper 2007-24-0030, 2007, doi: 10.4271/2007-24-0030.

Christensen, E., L. Fouts, G.M. Fioroni, R.L. McCormick, Private communication, March 2018.

Ding, C.P., M. Sjöberg, D. Vuilleumier, D.L. Reuss, X. He, and B. Böhm, "Fuel-film thickness measurements using refractive index matching in a stratified-charge SI engine operated on E30 and alkylate fuels", Experiments in Fluids (2018) 59: 59.

Fouts, L., G.M. Fioroni, E. Christensen, M. Ratcliff, R.L. McCormick, B.T. Zigler, S. Sluder, J.P. Szybist, J.E. Dec, P.C. Miles, S. Ciatti, J.T. Bays, W. Pitz, and M. Mehl. 2018. Properties of Co-Optima Core Research Gasolines. Technical Report NREL/TP-5400-71341. Golden, CO: National Renewable Energy Laboratory.

He, X., Y. Li, M. Sjöberg, D. Vuilleumier, C.P. Ding, F. Liu, and X. Li, "Impact of coolant temperature on piston wall-wetting and smoke generation in a stratified-charge DISI engine operated on E30 fuel", accepted for the Proceeding of the Combustion Institute.

Sjöberg, M. and W. Zeng, "Combined Effects of Fuel and Dilution Type on Efficiency Gains of Lean Well-Mixed DISI Engine Operation with Enhanced Ignition and Intake Heating for Enabling Mixed-Mode Combustion", SAE Int. J. Engines 9(2):750-767, 2016, doi:10.4271/2016-01-0689.

Sjöberg, M., D. Vuilleumier, N. Yokoo and K. Nakata, "Effects of Gasoline Composition and Octane Sensitivity on the Response of DISI Engine Knock to Variations of Fuel-Air Equivalence Ratio", COMODIA 2017, July 25 – 28, Okayama, Japan.

Zeng, W., M. Sjöberg, D.L., Reuss, and Z. Hu, "High-Speed PIV, Spray, Combustion Luminosity, and Infrared Fuel-Vapor Imaging for Probing Tumble-Flow-Induced Asymmetry of Gasoline Distribution in a Spray-Guided Stratified-Charge DISI Engine", Proc. Comb. Inst. 36:3, pp. 3459-3466, 2017, doi: 10.1016/j.proci.2016.08.047

Key Fiscal Year 2017 Publications

1. M. Sjöberg, X. He, "Combined effects of intake flow and spark-plug location on flame development, combustion stability and end-gas autoignition for lean spark-ignition engine operation using E30 fuel", International Journal of Engine Research, Vol 19, Issue 1, pp. 86 – 95, January 2018.
2. C.P. Ding, M. Sjöberg, D. Vuilleumier, D.L. Reuss, X. He, and B. Böhm, "Fuel-film thickness measurements using refractive index matching in a stratified-charge SI engine operated on E30 and alkylate fuels", Experiments in Fluids (2018) 59: 59.
3. C. K. Westbrook, M. Sjöberg and N.P. Cernansky, "A New Chemical Kinetic Method of Determining RON and MON Values for Single Component and Multicomponent Mixtures of Engine Fuels", Combustion and Flame, Vol. 195, pp. 50-62 (2018), doi: 10.1016/j.combustflame.2018.03.038
4. N. Van Dam, M. Sjöberg, and S. Som, "Large-eddy Simulations of Spray Variability Effects on Flow Variability in a Direct-injection Spark-ignition Engine Under Non-combusting Operating Conditions", SAE Paper 2018-01-0196.
5. X. He, Y. Li, M. Sjöberg, D. Vuilleumier, C.P. Ding, F. Liu, and X. Li, "Impact of coolant temperature on piston wall-wetting and smoke generation in a stratified-charge DISI engine operated on E30 fuel", accepted for the Proceeding of the Combustion Institute.
6. D. Vuilleumier, X. Huan, T. Casey and M. Sjöberg, "Uncertainty Assessment of Octane Index Framework for Stoichiometric Knock Limits of Co-Optima Gasoline Fuel Blends", accepted for SAE International Journal of Fuels and Lubricants.

Acknowledgements

The work was performed at the Combustion Research Facility, Sandia National Laboratories, Livermore, CA. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and

Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Acronyms, Abbreviations, Symbols, & Units

ϕ	Fuel-Air Equivalence Ratio
ϕ_m	Mass-Based Fuel-Air Equivalence Ratio
°CA	Crank Angle Degree
$[O_2]$	Oxygen Mole Fraction
BIT	Beijing Institute of Technology
DI	Direct Injection
DIB	Diisobutylene
DBI	Diffuse Back Illumination
DISI	Direct Injection Spark Ignition
EGR	Exhaust-Gas Recirculation
LED	Light Emitting Diode
PFI	Port-Fuel Injection
P_{in}	Intake Pressure
PM	Particulate Matter
PMI	Particulate Matter Index
MON	Motor Octane Number
NO_x	Nitrogen Oxides
RIM	Refractive Index Matching
rpm	Revolutions per Minute
RON	Research Octane Number
S	Octane Sensitivity
SNL	Sandia National Laboratories
$T_{coolant}$	Coolant Temperature
T_{in}	Intake Temperature