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Final CRADA Report – NFE-21-08852 Independent Fuel Property Effects of Fuel Volatility on Low Temperature Heat Release and Fuel Autoignition

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Buildings and Transportation Science Division

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ABSTRACT

This Cooperative Research and Development Agreement (CRADA) project between Argonne National Laboratory (ANL), Oak Ridge National Laboratory (ORNL), and Shell Global Solutions (Shell) was initiated as part of a Directed Funding Opportunity (DFO) call for proposals from the Co-Optimization of Fuels and Engines (Co-Optima) initiative funded by the Department of Energy (DOE). Shell had observed that volatile fuels suppress low temperature heat release (LTHR) more than expected based on the conventional gasoline autoignition metrics research octane number (RON) and motor octane number (MON). The role of LTHR contributes to autoignition phenomena for both boosted spark ignition (BSI) and advanced compression ignition (ACI) combustion modes. ACI combustion modes are applicable to large engines in the hard-to-electrify applications such as off-road, rail, and marine. Thus, having a reliable understanding of autoignition phenomena, including being able to accurately account for the effects of fuel volatility, is particularly important as new synthetic and bio-fuel compositions are considered.

This CRADA project aimed to test the hypothesis that the decreased LTHR is due to preferential evaporation of multicomponent fuels when using direct injection (DI) fueling technology, creating composition and reactivity stratification inside the combustion chamber. A custom set of fuels was designed and blended to test this hypothesis by Shell, with experimental engine studies at ORNL and engine combustion modeling by ANL. However, the initial experimental findings did not show the expected effect of fuel volatility suppressing LTHR. Instead, the LTHR propensity observed was independent of the fuel volatility.

Due to the unexpected experimental result, the remainder of the experimental effort was redirected to study the effect of fuel volatility on emissions under spark-ignited cold-start conditions. However, as with the LTHR experiments, the cold start effort did not show a meaningful effect of fuel volatility on cold start emissions. Meanwhile, improved engine CFD models have been developed for both LTHR and cold start operations for the Shell fuels with different volatilities. While the simulation efforts were not pursued further due to the insignificant effects of fuel volatility as shown in experiments, the models developed can be easily retooled for off-road, rail, and marine applications.

Statement of Objectives

This program aimed to fill knowledge gaps to better understand the impact of volatile fuels on LTHR, independent of RON and MON. In particular, the work was planned to test the hypothesis that preferential evaporation of volatile components in DI engines produces reactivity stratification such that the less reactive volatile components govern the overall reactivity. The work was structured such that each organization in the CRADA played a critical role to test the hypothesis and understand the underlying phenomena: Shell was to develop a custom set of fuel blends that vary fuel volatility independent of RON and MON, ORNL was to experimentally measure LTHR in a highly instrumented research engine, and ANL was to model the data generated by ORNL to develop a better understanding of the applicable physical phenomena.

Benefits to DOE Vehicle Technologies Office Mission

This CRADA project was competitively awarded by the DOE Vehicle Technologies Office (VTO) as part of the Co-Optima initiative. The Co-Optima initiative aimed to co-develop fuels and engines in an effort to maximize energy efficiency and the utilization of renewable fuels. This included understanding the role of fuel properties on engine performance and emissions under both BSI operating conditions and higher efficiency ACI combustion modes. This CRADA project was designed to further this understanding by focusing on fuel volatility, as measured by vapor pressure. Vapor pressure was not a major focus within the Co-Optima initiative, thus this CRADA project aimed to fill the knowledge gap by determining the independent role of this fuel property in engine efficiency.

Technical Discussion

Shell produced and shipped to ORNL six matched-pair custom fuel blends: 6 low volatility fuels (LVFs) and 6 high volatility fuels (HVFs). HVFs were prepared by blending light ends (butanes and butenes) into the corresponding LVF to give a 20-25 kPa increase in Reid vapor pressure (RVP). Shell provided key fuel properties as well as detailed hydrocarbon analysis (DHA) data to assist engine testing and CFD modeling. Key fuel properties and fuel composition differences are shown in Table 1 with the blue and red highlighting the low and high volatility blends, respectively, and the green highlighting the major blend component.

Table 1. Matrix of custom fuel blends produced by Shell and sent to ORNL to vary fuel volatility while holding RON and MON roughly constant.

	Aromatic		Ethanol		Prenol		Diisobutylene		Cyclopentane		Carbonate	
	LVF	HVF	LVF	HVF	LVF	HVF	LVF	HVF	LVF	HVF	LVF	HVF
RON (-)	98.2	97.8	99.8	99.8	97.9	98	97.7	97.6	97.5	97.7	96.8	96.8
MON (-)	89.4	90	89.6	89.7	87.4	87.5	88.5	88.5	88.3	88.8	89.5	89.7
RVP (kPa)	51.6	78	55.3	75.5	49.8	75.8	52.4	76.3	59.2	75.5	51	76.5
Aromatic (vol%)	20	20	10	10	10	10	10	10	10	10	10	10
Ethanol (vol%)	0	0	10	10	0	0	0	0	0	0	0	0
Prenol (vol%)	0	0	0	0	10	10	0	0	0	0	0	0
DIB (vol%)	0	0	0	0	0	0	10	10	0	0	0	0
CPT (vol%)	0	0	0	0	0	0	0	0	10	10	0	0
Carbonate (vol%)	0	0	0	0	0	0	0	0	0	0	10	10

A series of experiments were conducted to test the hypothesis that higher fuel volatility suppresses LTHR due to preferential evaporation. Experiments were conducted to investigate both port fuel injection (PFI) and DI fuel injection with fuels differing in volatility but with otherwise matched fuel properties and composition. ORNL started this effort with the high aromatic LVF and HVF from Table 1. This experiment was conducted at a condition which ORNL had previously demonstrated was conducive to LTHR [1]: 1500 rpm with constant air and fuel rate and very late combustion phasing with combustion midpoint (CA50) at 40-50 crank angle degrees (CAD) after top dead center (aTDC). The intake air temperature was varied between 35 and 100 °C, the air-to-fuel ratio was varied from stoichiometric (lambda = 1.0) to fuel-lean (lambda = 1.2), and the resultant indicated mean effective pressure (IMEP) was 16.3-17.8 bar.

The cylinder pressure and heat release rate from these experiments at an intake temperature of 80 °C are shown in Figure 1. At all three air-to-fuel ratios, LTHR can be observed for the PFI fueling, and it becomes more prominent as the air-to-fuel ratio becomes fuel lean. For the DI fueling, LTHR is significantly less pronounced, but begins to appear as the mixture becomes more fuel lean. Despite these observations, no significant differences were observed between the low and high volatility fuels. Thus, it was concluded that, at this condition, the main drivers were the fueling type (PFI vs. DI), which can affect charge cooling, and the air-to-fuel ratio. Fuel volatility has a minor effect if any.

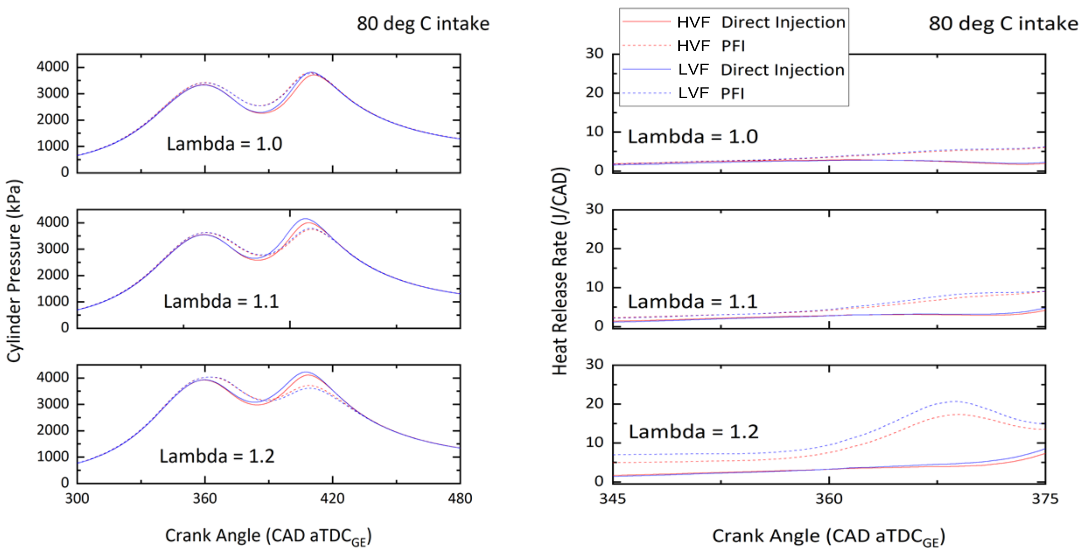

Figure 1. Cylinder pressure and heat release rate for the aromatic LVF and HVF at an engine speed of 1500 rpm, fuel rate of 44.5 g/min, an intake temperature of 80 °C, and air-to-fuel ratios of lambda = 1.0, 1.1, and 1.2.

In parallel, CFD efforts from ANL were initially focused on investigating fuel volatility effects under the LTHR operating condition previously used in Co-Optima. To accurately account for preferential evaporation effects, an improved CFD model for the ORNL engine was developed building on ANL's prior Co-Optima work [2]. The engine CFD model uses the G-equation model for capturing turbulent flame propagation and the finite rate well-stirred reactor model for predicting low-temperature reactions in the unburnt gas. Instead of using the default single-component evaporation model, a multi-component evaporation model was incorporated in the engine CFD model to capture the preferential evaporation behavior of the lighter fuel components. The model was first tested for multi-cycle CFD simulations for the Co-Optima Alkylate fuel under a LTHR engine operating condition with strong pre-spark heat release (PSHR). As shown in Figure 2, the mean in-cylinder pressure and apparent heat release rate (AHRR) traces predicted using the multi-component evaporation model are slightly higher than that predicted using the single-component evaporation model, highlighting the non-negligible role of preferential evaporation in affecting LTHR. Multi-cycle engine simulation setups were then created for the same operating conditions as the ORNL experiments with select Shell fuels. In particular, three fuels were selected for this analysis: baseline gasoline containing 10% ethanol (E10), and the ethanol LVF and HVF fuels shown in Table 1. The surrogate for baseline E10 fuel was previously developed by Lawrence Livermore National Laboratory for the Partnership to Advance Combustion Engines (PACE) consortium. The surrogates for the LVF and HVF ethanol fuels in Table 1 were created subsequently by blending ethanol and the light end components into the baseline E10 surrogate, informed by the detailed hydrocarbon analysis (DHA) data provided by Shell. However, the LTHR simulation effort for the Shell fuels was not pursued further based on the new ORNL experimental results.

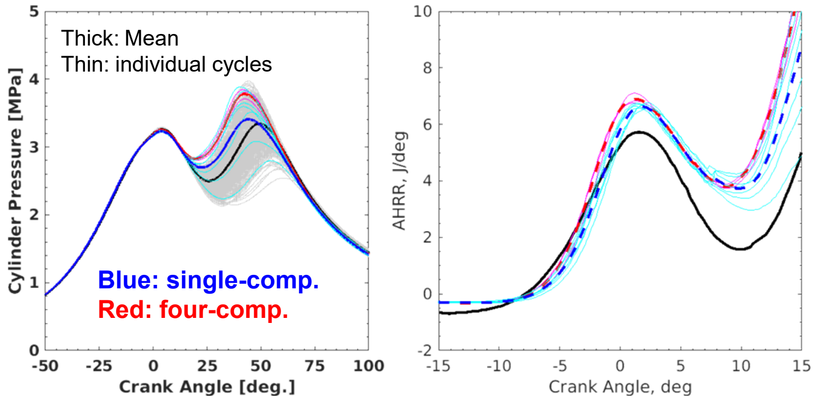

Figure 2. CFD prediction of in-cylinder pressure and heat release rate traces using single-component and multi-component evaporation models, respectively, in comparison with experimental data (black solid lines) for the Co-Optima Alkylate fuel under a strong pre-spark heat release (PSHR) engine condition.

After reviewing these results, Shell requested that the high load testing be discontinued and the remaining project resources be redirected to investigate the effect of fuel volatility on engine cold-start emissions. ORNL had previously performed cold start experiments as part of the PACE consortium. As a result, the experimental facilities were in place and the methodology to perform these experiments was established [2, 3]. Thus, the project was redirected to focus on cold start emissions after obtaining approval from DOE VTO.

Experiments were conducted at a stoichiometric steady-state engine operation at 1300 rpm and 2 bar net IMEP. This speed/load condition was determined as a steady-state surrogate for the catalyst heating portion of the cold-start operation by the U.S. DRIVE Advanced Combustion and Emission Control Technical Team, which included input from US light-duty-engine manufacturers. During these experiments, engine coolant, oil, and intake air were all controlled to 20 °C to simulate the engine boundary conditions at cold start. During cold start operation, it is desirable to increase the exhaust enthalpy (or heat content) as much as possible, quantified as kW/L engine displacement. This is accomplished by retarding combustion phasing as much as possible, which is aided by using multiple fuel injections.

Figure 3 shows the gaseous emissions results from the aromatic LVF and HVF shown in Table 1. The results show that both unburned hydrocarbon and NOx emissions change significantly with exhaust enthalpy and are dependent on the number of fuel injections. However, the effect of fuel volatility between the fuels is very small and within the uncertainty of the experimental measurements. Experimental results were collected with two additional fuels, and in all cases, fuel volatility did not cause any significant difference in emissions.

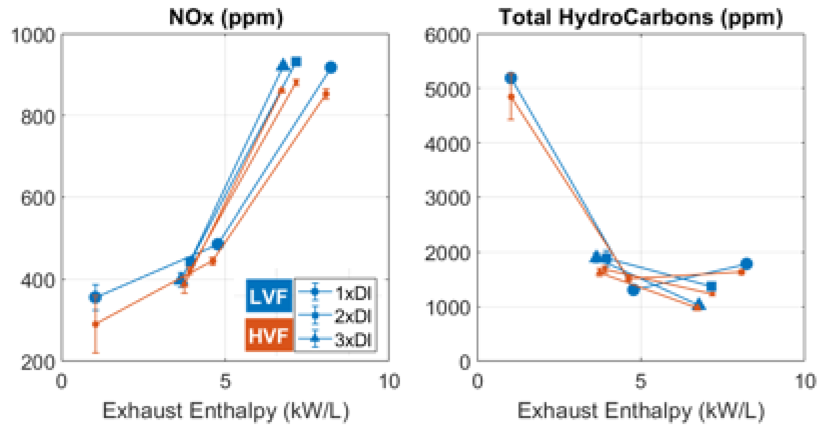

Figure 3. Nox and unburned hydrocarbon emissions from the cold start test using the aromatic LVF and HVF shown in Table 1.

To investigate the fuel volatility effect on engine cold-start emissions, new engine simulations using the G-equation model were designed and performed by ANL for cold start operations. As the engine CFD model was originally developed for LTHR operations, the model was re-calibrated using the ORNL data with the baseline gasoline surrogate. Figure 4 shows the pressure traces from two CFD simulations using two different values for b_1—a model constant in the G-equation model—in comparison with experimental data (spark timing of -10 CAD). The original model calibrated for the LTHR operation with b_1=1.5 significantly over-predicts peak pressure. Reducing this model constant to b_1=1 provides satisfactory prediction of the pressure trace and flame propagation dynamics. The newly calibrated model was then used to set up simulations for the LVF and HVF ethanol fuels shown in Table 1 fuels. Simulations progressed but did not proceed further as the new experimental results suggested fuel volatility has little impact on emissions.

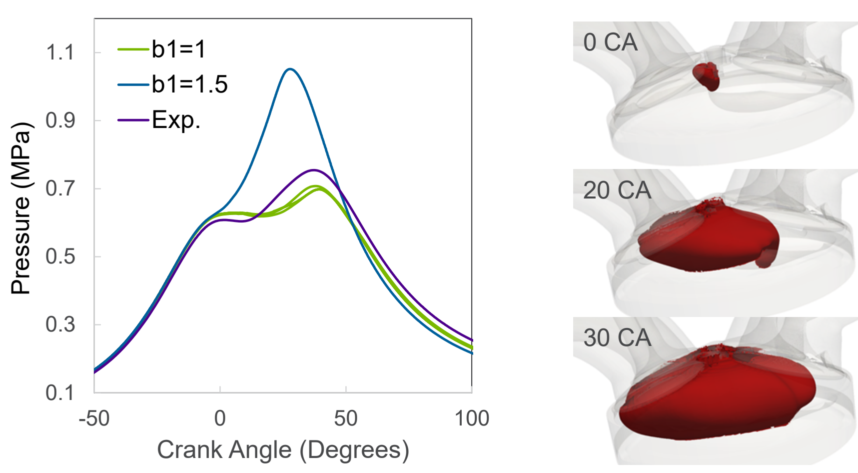

Figure 4. Left: Pressure traces from two CFD simulations obtained using different values for b1 (a model constant in the G-equation model), in comparison with experimental data. Right: Temperature isocontour (T=1500 K) at different crank angles for the "b_1=1" case.

Subject Inventions

No inventions were made as part of this CRADA.

Commercialization Possibilities

No commercialization is expected as a result of this CRADA.

Plans for Future Collaborations

No future collaborations are currently planned as an outcome of this CRADA.

Conclusions

A CRADA project between ANL, ORNL, and Shell was carried out to better understand the effect of fuel volatility on LTHR. Specifically, the study was designed to test the hypothesis that high volatility fuels suppress LTHR in DI engines, independent of RON and MON, due to preferential evaporation. The role of Shell was to design a fuel matrix that held RON and MON constant while changing fuel volatility, while ORNL was to experimentally measure LTHR in a highly instrumented research engine, and ANL was to model the physical phenomena.

However, the initial experimental results from ORNL showed no effect of fuel volatility on LTHR. Instead, the LTHR propensity was dominated by fueling type (PFI vs. DI) and by the air-to-fuel ratio. The remaining project resources were redirected to investigate the role of fuel volatility on emissions during cold start. However, as with the LTHR measurements, there were no significant differences in emissions that could be attributed to fuel volatility. Based on the results of this CRADA project, it can be concluded that fuel volatility does not have a significant impact on either LTHR or cold start emissions.

References

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Acronyms

ACI	Advanced compression ignition
ANL	Argonne National Laboratory

aTDC	After top dead center
BSI	Boosted spark ignition
CA50	Combustion midpoint
CAD	Crank angle degrees
CRADA	Cooperative research and development agreement
DFO	Directed funding opportunity
DI	Direct injection
E10	Gasoline containing 10% ethanol
HVF	High volatility fuel
IMEP	Indicated mean effective pressure
LTHR	Low temperature heat release
LVF	Low volatility fuel
MON	Motor octane number
ORNL	Oak Ridge National Laboratory
PACE	Partnership to Advance Combustion Engines
PFI	Port fuel injection
RON	Research octane number
VTO	Vehicle Technologies Office