LAWRENCE LIVERMORE NATIONAL LABORATORY

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Small Volume Fuel Testers Report

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Small Volume Fuel Testers Report (old FY16 Task G.1.2)

1. Background

Principal Investigator: Ingmar Schoegl (LSU)

Team Members: Pawan Sharma (LSU; graduate student)

FY16 Funding: $74,999 + $15,000 for on-site visit at LLNL (Oct-Dec 2016).

2. Summary

Micro-liter fuel ignition testing (μ-FIT) is based on the premise that characteristics FREI (Flames with Repetitive Extinction and Ignition, i.e. cyclically occurring combustion events within heated capillaries), are linked to fuel properties. In early FY16, proof-of-concept measurements with primary reference fuel (PRF) mixtures, i.e. blends of n-heptane and iso-octane, yielded clear evidence for the feasibility of the approach. Our experiments showed that it is critical to accurately link observed flame positions to local temperatures, which provides information on ignition, extinction and flame propagation, all of which are known to be impacted by fuel properties. In FY16, one major hurdle was uncertainty of temperature calibration, which required significant efforts for corrective action that were not included in the original scope of work. Temperature calibrations are obtained by translating a thermocouple within the capillary in absence of a flame. While measurements have good repeatability when accounting for transient and insertion effects, results from nominally identical thermocouples reveal unacceptable uncertainty (up to ±50K), which is attributed to variations in thermocouple placement and manufacturing tolerances. This issue is currently being resolved by switching to non-intrusive optical temperature measurements. Updates are expected to yield uncertainties of less than ±10K, while also eliminating transient and insertion effects. The experimental work was complemented by computational efforts where it was shown that a simplified Lagrangian zero-D model with detailed kinetics yields fuel-specific differentiation of ignition temperatures for simple fuels that are consistent with experiments. Further, a 2D transient model was implemented in OpenFOAM to investigate combustion behavior of simple fuels at elevated pressure. In an upcoming visit to LLNL, more advanced simulations using LLNL's computational tools (e.g. zero-RK) are planned, which will yield additional numerical insights on FREI behavior of more realistic spark ignited (SI) engine fuel surrogates. As there is a lag between DOE FY16 and the time frame of the LSU subcontract, it is anticipated that deliverables outlined in the scope of work will be met by the end of the subcontract (January 2017).

3. Performance

a) Big picture - do we know what the results experimental results mean and how they connect to the relevant Co-Optima objectives?

The μ-FIT experiment aims to augment and/or replace existing fuel testing standards, e.g. RON/MON for SI engine fuels, which is especially important for the selection of fuel feed stock candidates at a stage when only small quantities are available. Specifically, the μ-FIT experiment yields information on ignition, flame propagation, and extinction which are, respectively, linked to auto-ignition, flame speed, and pre-ignition resistance (via critical flame kernel diameter and quenching distance). One complicating factor are non-adiabatic boundaries, which require correlation and/or compensation in order to compare to established techniques.

b) What is the applicability of the results of the small volume testing rigs to combustion phenomena at engine-relevant conditions (including boosted SI and ACI strategies > 20 bar)?

To date, all μ-FIT experiments have been conducted at atmospheric pressure. While correlations for pressure variations are available in literature, they are not expected to account for shifts in kinetic pathways. A better approach involves conducting μ-FIT experiments at elevated pressure, where results can be correlated to results from shocktube and/or rapid compression machines. Moderate pressure increases (2-5 bars) are feasible within FY17. 2D numerical results from FY16 indicate that FREI will show similar propagation characteristics, although extinction temperatures will decrease. Experimental results are expected to provide guidance for required steps to further increase pressures towards engine-relevant pressures. Specifically, requirements for reduced capillary diameters to counteract reductions of the quenching diameter will be investigated.

c) How do the measurements connect to inputs to the Engine Merit Function(s)?

Measurements from μ-FIT are connected to the Engine Merit Function via octane numbers and flame speed. Proof-of-concept measurements show a clear connection between μ-FIT results and both PRF octane rating and flame speeds. Upcoming experiments with TRF blends (n-heptane/iso-octane/toluene) will clarify impact of fuel sensitivity on μ-FIT results. In terms of theory, ignition temperatures can be related to ignition delays using the Livengood-Wu integral although the impact of low temperature kinetics needs to be scrutinized.

d) How accurate are the results (e.g., +/- 0.1, 1, or 10 RON; % relative error in ignition delay or flame speed)?

Available experiments with PRF blends (0/50/100 RON) indicate that correlations to extinction temperatures show the most pronounced sensitivity. Results indicate a linear trend, where the slope is assessed as 1.0-1.5 Kelvin per unit RON based on a curve fit of multiple tests at a given pressure. With improved liquid fuel delivery, uncertainties of curve fits are expected to be less than 5 K, which translates into accuracies of single digit RON. Increased accuracies are expected by using measurements at multiple pressures. Flame speeds and PRF results reveal similar linear correlations with extinction temperatures; slopes up to 30 Kelvin per cm/s indicate that relative errors of less than 1% are achievable.

e) In what timeframe could results be provided to the LGGF team?

For high vapor pressure fuels available at quantities in the order of 10ml, tests using improved fuel delivery and moderate pressures are possible with relatively modest effort (i.e. within FY17 and current funding levels). Delivery systems for smaller quantities of potentially lower vapor pressure fuels are more difficult and require more effort, especially as shifts towards higher pressure work are anticipated.

f) Are any major facility investments required?

Continuous improvement of the μ-FIT concept is possible at current funding levels without major facility investments. However, the PI is currently pursuing substantially larger funds from the DOE/EERE university program (DE-FOA-0001461). If successful, increased funds will allow for more rapid development of μ-FIT, including high pressure work and micro-liter fuel delivery and characterization.

g) What is the expected throughput (fuels/month)?

Within FY17, one fuel per day is anticipated after full resolution of temperature uncertainty and implementation of improved fuel delivery. Long-term, test durations of approximately 1 hour for a full fuel characterization test are targeted. This estimate corresponds to 5 fuels/day or 100 fuels/month running at maximum capacity. Estimates are based on tests where combustion phenomena are assessed at around 20 test conditions each at multiple pressures and/or equivalence ratios. Currently, each test takes approximately 90 seconds and involves imaging of the flame as well as recording of pressure traces. Times required for individual tests can be shortened by automation (~10 seconds), whereas the number of tests can be reduced by design of experiment once the parameter space is fully understood.

h) What is the expected volume of fuel required?

Short-term, approximately 10 ml after an initial revision of the fuel delivery system. Long-term, 20 μl with micro-liter fuel delivery system (see DOE/EERE university program DE-FOA-0001461). Standard shipping & handling requirements of flammables apply (i.e. same as for commercial suppliers).

3. FY16 Accomplishments and Highlights

- Delivered proof-of-concept for octane number and flame speed sensitivity of μ-FIT measurements.
- Identified sources of measurement error and uncertainty and took corrective action.

- Conducted tests with sapphire capillaries that exhibit better temperature performance and have potential benefits for work at elevated pressures.
- Illustrated auto-ignition order of different gaseous fuels based on 0D transient work (Cantera) as a validation of experimental observations.
- Illustrated pressure dependency of FREI characteristics using 2D simulations (OpenFOAM), indicating that extinction temperatures are strongly affected through changes in quenching diameters.

4. Publication/Presentation List

Manuscript (in revision): I. Schoegl, P. Sharma and M. J. McNenly. *Ignition and extinction of gaseous fuels in the FREI regime*.

5. Appendix/Supplementary Material (feel free to add any presentations, papers, etc.)

N/A.