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Optical Fuel-Air Sensor

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Interim Report**

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14. ABSTRACT LIBS, or <i>laser-induced breakdown spectroscopy</i> , is a widely used diagnostic enabling “stand-off” detection of atomic components of parent constituents; it involves the use of a pulsed laser that induces dielectric breakdown of the target media/sample and collection of the emitted radiation from the laser spark. Typically, LIBS is employed to analyze solid samples. The focus of this project is advancement of LIBS for analysis of gaseous media for the specific purpose of Fuel-Air (F/A) sensing, to derive the local F/A ratio within a high-speed combustor. For this program, our goals are to 1) improve the accuracy of the measurement technique (i.e., of the F/A ratio) and 2) improve the usability of the technique. To improve accuracy (and satisfy Goal 1), we are focusing on the use of Machine Learning to analyze the emission spectra. For Goal 2 we are exploring various improvements to the technique that include miniaturization of the needed equipment (e.g., the laser) and approaches to shutter the laser pulse to reduce the pulse energy for dielectric breakdown and thus the likelihood of window damage.			
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Abstract

LIBS, or *laser-induced breakdown spectroscopy*, is a widely used diagnostic enabling “stand-off” detection of atomic components of parent constituents; it involves the use of a pulsed laser that induces dielectric breakdown of the target media/sample and collection of the emitted radiation from the laser spark. Typically, LIBS is employed to analyze solid samples. The focus of this project is advancement of LIBS for analysis of gaseous media for the specific purpose of Fuel-Air (F/A) sensing, to derive the local F/A ratio within a high-speed combustor. For this program, our goals are to 1) improve the accuracy of the measurement technique (i.e., of the F/A ratio) and 2) improve the usability of the technique. To improve accuracy (and satisfy Goal 1), we are focusing on the use of Machine Learning to analyze the emission spectra. For Goal 2 we are exploring various improvements to the technique that include miniaturization of the needed equipment (e.g., the laser) and approaches to shutter the laser pulse to reduce the pulse energy for dielectric breakdown and thus the likelihood of window damage.

Progress as of Aug 2021

LIBS stands for *laser-induced breakdown spectroscopy* and is a widely used method used for “stand-off” detection of atomic components of parent constituents. It is often used to analyze solid samples rather than gaseous samples, which is our focus.

Three results from the first year of progress are summarized below.

1. A concerted effort was made to complete a study employing LIBS and advanced numerical simulations from our Research Cell 19 cavity flameholder. The end results of this study are summarized as follows.
 - a. We showed that two LIBS datasets employing different laser systems were almost identical.
 - b. We showed the relative importance of the density of “calibration points” on the derived fuel-air ratios and density.
 - c. We demonstrated good (even excellent) agreement in comparison with the high-fidelity simulations under non-reacting conditions (but some disagreement in the shear layer).
 - d. We showed that four reduced kinetic models produced a substantial range of results (e.g., temperatures and reaction progress), highlighting the importance of a validated diagnostic technique like n-LIBS for model testing.
2. A principal goal of this program was to improve analysis approaches of the LIBS spectra in deriving fuel-air ratios and gas density. While a few methods for improved analysis were discussed, a completely new method arose from our partners at Seoul National University: use of machine learning to reduce spectra. This approach was tested on sample data collected previously in the Room 14 variable pressure combustion chamber, and the results demonstrated the efficacy of the approach. Indeed, in previous work, we routinely subtracted broadband plasma emission before attempting to analyze the spectra

(composed of atomic lines from the original parent molecules), but via machine learning it was shown that the broadband emission intensity is strongly related to the gas density. The predictive performance of the machine-learning model was validated by predicting both fuel-air ratio and density in the sample data.

This represents the first time machine learning has been applied to LIBS analysis of gaseous samples.

3. An old 30-Hz Nd:YAG laser system (that was not working originally) acquired from RQT was repaired and then upgraded with an injection seeder (to improve the uniformity of pulses produced by the laser). As our other LIBS laser systems operate at 10 Hz repetition rate, this repaired/upgraded system will be a valuable addition to our LIBS instruments.

Papers published from this effort are as follows.

1. McGann, B., Ombrello, T.M., Peterson, D.M, Hassan, E., Hammack, S.D., Carter, C.D., Lee, T., and Do, H., Lean fuel detection with nanosecond-gated laser-induced breakdown spectroscopy, *Combust. Flame* **224** (Special Issue), 209 (2021).
2. Lee, J., McGann, B., Hammack, S.D., Carter, C., Lee, T., Do, H., Bak, M.S., Machine learning based quantification of fuel-air equivalence ratio and pressure from laser-induced plasma spectroscopy, *Optics Express* **29**, 17902 (2021).