



Automotive Low Temperature Gasoline Combustion Engine Research

Isaac Ekoto & Richard Steeper
Sandia National Laboratories

2014 DOE Vehicle Technologies Annual Merit Review
Arlington, VA
June 17, 2014

Program Manager: Leo Breton & Gurpreet Singh
DOE Office of Vehicle Technologies

Project ID: ACE006

This presentation does not contain any proprietary, confidential, or otherwise restricted information



Overview

Timeline

- Project provides fundamental research supporting DOE/industry advanced engine development projects.
- Project directions and continuation are evaluated annually.

Budget

- Project funded by DOE/VT
- FY13 funding: \$680k
- FY14 funding: \$670k

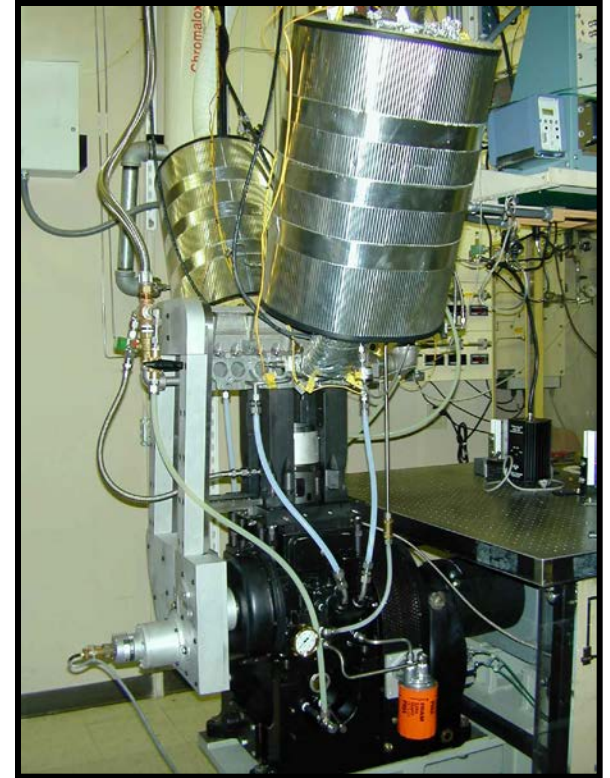
Barriers identified in VT Multi-Year Program Plan

- Inadequate fundamental knowledge of engine combustion:
 - Fuel injection, evaporation, and mixing;
 - Heat transfer and thermal stratification;
 - Ignition, low-temperature combustion, and emissions formation.
- ACEC 2013 targets for Advanced Combustion R&D (2020):
 - A 20% improvement in engine efficiency, compared to a 2010 baseline.
 - Engines are commercially viable and meet 2020 emissions standards.

Partners

- Project lead: Isaac Ekoto, Sandia
- Industry Partners:
 - GM, Ford, & Chrysler: technical guidance
 - 15 Industry partners in DOE Working Group.
- University/National Lab Collaborators:
 - Oak Ridge National Lab:
 - Joint negative valve overlap (NVO) fueling experiments
 - Lawrence Livermore National Lab:
 - Chemical analysis, chemical kinetics models
 - Lawrence Berkeley National Lab:
 - Detailed engine sample speciation
 - Argonne National Lab:
 - Joint ignition experiments & modeling
 - USC:
 - Transient plasma advanced ignition system research

- »Perform experiments in an optical engine equipped and configured for automotive LTGC combustion strategies.
- »Develop and apply diagnostics to acquire in-cylinder measurements of fundamental physical processes.
- »Apply suite of computer models to guide and interpret engine experiments.
- »Leverage knowledge gained through technical exchange with DOE Vehicle Technologies program participants.



»Motivation for automotive LTGC research:

1. NVO operation has been identified by automotive OEMs as a viable pathway for SI mixed-mode engines:

- High-specific-output stoichiometric operation at high load.
- **High-O₂** NVO enables low-load LTGC through improved charge heating & chemistry enhancement.
- **Low-O₂** NVO improves charge reactivity through fuel reforming.
- Advantages demonstrated, but chemical & physical details are poorly understood.

2. Advanced ignition systems can enhance combustion & enable increased charge dilution. Potential advantages include:

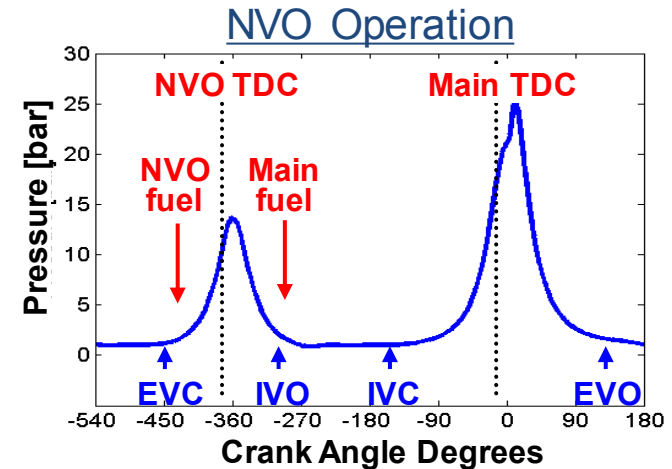
- Improved engine stability and lower misfire rates.
- Lower energy consumption for highly boosted cylinders.
- Less sensitivity to charge motion.

»Overall objective:

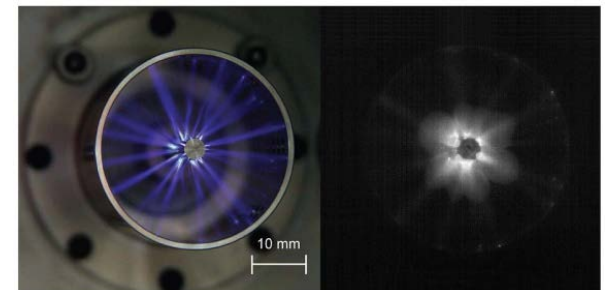
- Expand fundamental understanding of automotive LTGC processes needed to achieve clean and fuel-efficient engines.

»Specific objectives:

- Characterize NVO products that impact main combustion.
- Develop, validate, and apply predictive LTGC models.
- Perform exploratory advanced ignition research and upgrade the vacated engine lab for more dedicated experiments.



Advance Ignition Systems (e.g., Low Temperature Plasma)



Singleton et al, J Phys D Appl Phys, 2011;44.

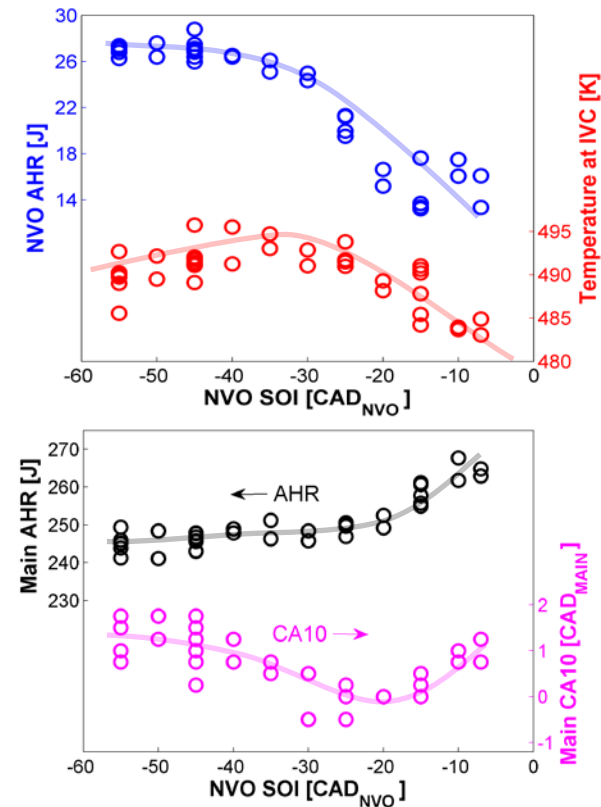
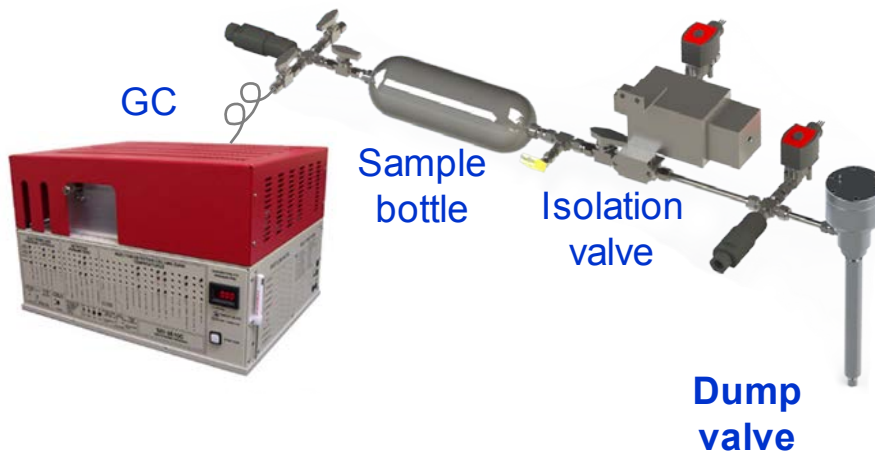


Milestones

»FY14 accomplishments are divided into **four** topics:

1. Analysis of **high-O₂** NVO cylinder sampling experiment results w/ important species identified.
 - Milestone: Demonstrate capability to speciate NVO products via the dump-valve & Gas Chromatograph apparatus
 - Milestone: Apply Chemkin-Pro model of main combustion to clarify NVO chemistry enhancement.
2. Speciation of **low-O₂** NVO products in support ORNL fuel reforming strategies.
 - Milestone: Quantify extent of rich combustion for late-injection NVO fueling.
3. Initiation of vacuum ultraviolet (VUV) mass spec experiments at the LBNL synchrotron for detailed NVO sample speciation.
 - Validate GC measurements & identify unique species
4. Development of new opportunities for advanced gasoline ignition.
 - Milestone: Complete survey of advanced gasoline ignition challenges & opportunities.
 - Milestone: Begin upgrades of lab hardware for a vacated engine lab to accommodate advanced ignition testing.

- » With NVO start of injection (SOI) retard the NVO heat release & main (IVC) charge temperatures decrease:
 - Reduced residence time for NVO reactions to take place
 - Increased piston wetting
- » Conventional expectation is an adverse impact on main combustion; however:
 - Main-combustion heat release increases w/ NVO SOI retard
 - CA10 generally advances
- » It is known that chemistry effects can enhance reactivity.
 - Dump sampling apparatus designed & implemented in FY13 to characterize NVO product composition and illuminate these chemical effects ...



Operating conditions:

- NVO: 150 CAD; RGF ~ 50%
- $T_{\text{Intake}} = 120^\circ\text{C}$; $T_{\text{EVC}} = 404^\circ\text{C}$
- Isooctane split inject: 1.2 + 8.4 mg
- NVO O_2 : 7%
- $\phi_{\text{Main+NVO}} = 0.65$
- IMEP = 190 kPa; COV < 3%

- » Retarded NVO SOI decreased CO₂ & increased CO; consistent w/ observed locally rich NVO combustion.
 - Excellent agreement w/ prior CO laser-absorption measurements.

Fitzgerald & Steeper, *SAE Int J Engines* 3(2):396-407, 2010.

- Baseline data shows increased CO (and HC) was due to NVO reactions.
- » Isooctane & large HC intermediate profiles were largely insensitive to NVO SOI.
- » Smaller HC species have stronger sensitivity to NVO SOI.

▪ Ethane:

- Late NVO SOI values roughly double relative to Early NVO SOI values.

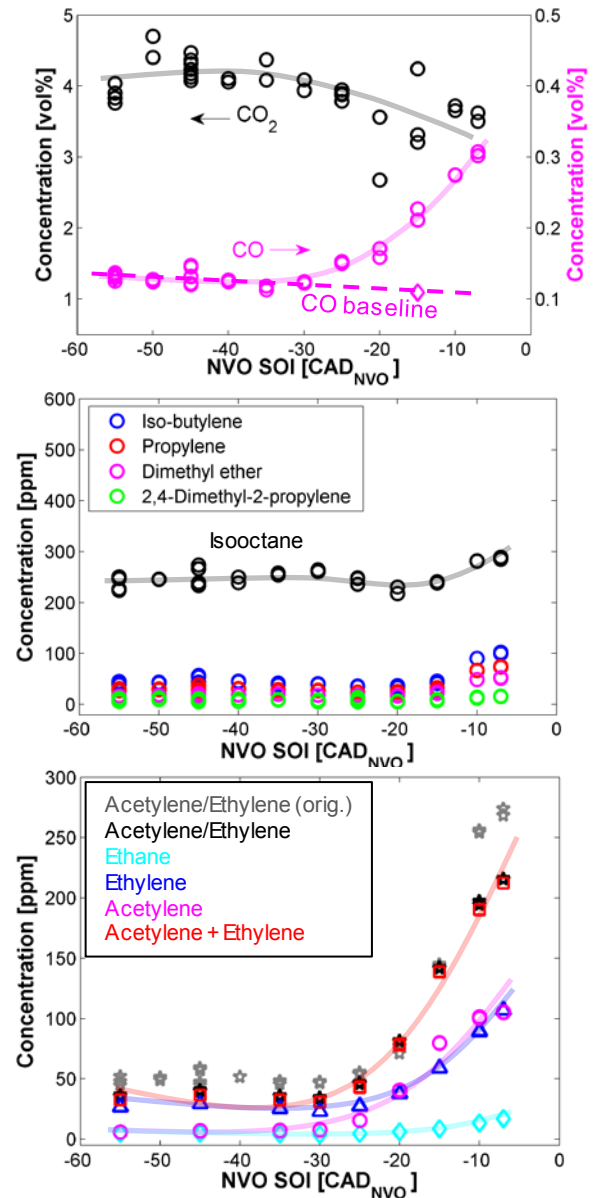
▪ Acetylene/Ethylene:

- New GC column enables acetylene/ethylene differentiation; results agree well w/ earlier combined measurements.
- Acetylene already identified as an important species that enhances main charge reactivity.

Puranam & Steeper, *SAE Int J Engines* 5(4):1551-60, 2012.

- Rapid rise (starting around -20 CAD_{NVO}) coincides w/ increased main HR.

We can now unambiguously identify increased acetylene production as NVO SOI is retarded.





Technical accomplishment 1: **High-O₂ NVO Experiments**

Single-zone combustion modeling w/ inputs from sample speciation.

»Chemkin-Pro w/ LLNL detailed isooctane mechanism

- FY13 modeling approach updated w/ composition assigned from FY14 GC measurements.
- Engine geometry, pressure, & temperatures at IVC applied

»Early NVO SOI:

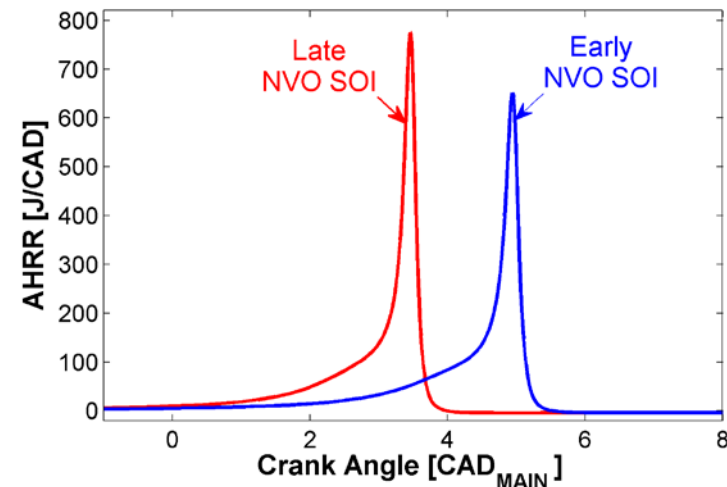
- Intake temperature offset 46 K to match experiment CA10.

»Late NVO SOI:

- Approximate 2-CAD phasing advance for Late NVO SOI was well reproduced by the simulations.
- The impact on main combustion phasing from small HCs & H₂ was systematically evaluated:
 - Acetylene responsible for **83%** of the phasing advance.
 - Hydrogen responsible for most of remainder.
 - Ethylene had a neutral effect.
 - Methane slightly retarded main phasing.

Measured species concentrations:

Species	Early NVO	Late NVO
Hydrogen	61.1	528 ppm
Methane	70.4	304 ppm
Acetylene	11.8	128 ppm
Ethylene	47.1	128 ppm
DME	21.6	49.2 ppm



Model results confirm the main combustion phasing **chemical effect** is mostly due to improved charge reactivity from **increased NVO acetylene production**.

Technical accomplishment 2: **Low-O₂ NVO Experiments**

Reproduced ORNL low-O₂ NVO experiments & measurements

»Initial NVO O₂ & bulk gas temperatures closely matched.

»Key hardware features:

	ORNL	SNL
Operation & sample strategy	Unique 6-stroke cycle & valve strategy	Dump-valve system
Diagnostics	FTIR	GC
Injector	Side-mounted DI	Central mounted DI
Displacement [L]	0.5	0.633

▪ NVO temperature and inlet O₂ concentration closely matched

»Unlike high-O₂ NVO, H₂ & HC production increase w/ earlier NVO SOI.

▪ CO trends are well matched.

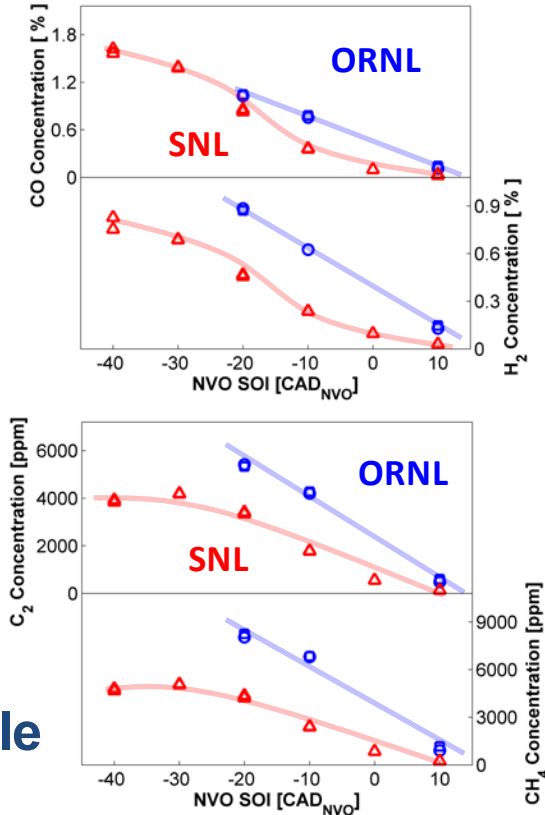
▪ SNL data has a distinct offset for a fixed NVO SOI.

▪ Bulk-gas reformation appears to be the driving mechanism rather than fuel surface reactions.

»Substantially larger values of C₂ species produced by low-O₂ NVO relative to high-O₂ NVO.

Operating conditions SNL Engine:

- NVO: 150 CAD; RGF ~ 50%
- T_{Intake} = 90 °C; T_{EVC} = 452 °C
- Isooctane split inject: 2.0 + 11.6 mg
- NVO O₂: 3%
- $\phi_{\text{Main+NVO}} = 0.85$
- IMEP = 290 kPa; COV < 1%

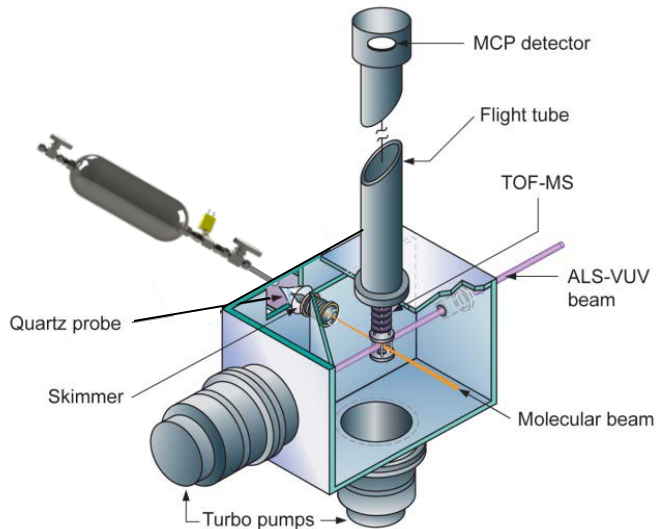


Low-O₂ NVO potentially represents a **more controllable pathway** to optimal HC intermediate production.

Technical accomplishment 3: **VUV Molecular Beam Mass Spec** Initiated exploratory experiments at LBNL synchrotron

» Leveraged existing SNL flame measurement capability to characterize NVO product species:

- Synchrotron radiation photo-ionizes sample molecules
 - Continuous & tunable soft X-ray beam (7.8 to 17 eV)
 - "Soft ionization" limits fragmentation for unambiguous identification.
- Species measured by time-of-flight mass spec
 - Isomer identification possible from photo-ionization energy (PIE) curves
- Flat-flame (McKenna burner) replaced by the sample bottles transported from Sandia — **45 minutes away**.



» Obj. 1: Detailed **high-O₂** NVO product speciation:

- Validate GC measurements
 - Measure species that cannot be quantified by the GC (e.g., aldehydes, isomers, or species that co-elute)
- Generate parametric database for improved NVO modeling
- Identify NVO product species that impact main combustion

» Obj. 2: Detailed **low-O₂** NVO product speciation:

- Confirm ORNL results obtained w/ different sampling technologies
- Identify NVO product species that impact main combustion

Represents a powerful new capability for detailed sample speciation.

Technical accomplishment 3: VUV Molecular Beam Mass Spec

Initial measurements of acetylene, ethylene, & isooctane

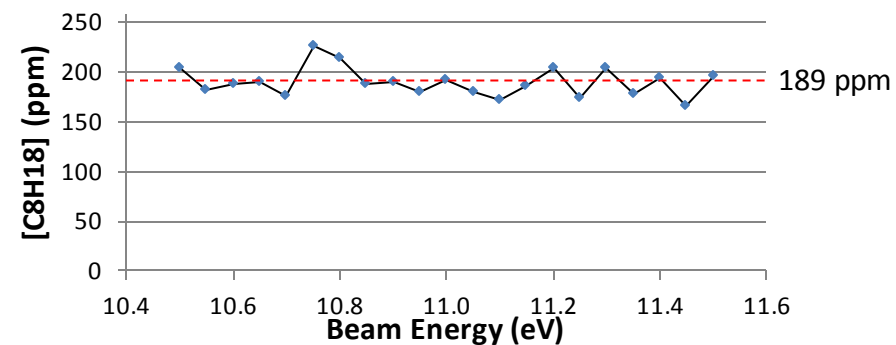
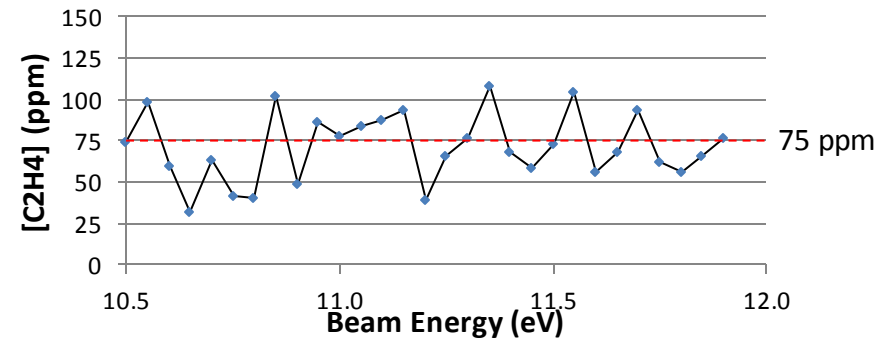
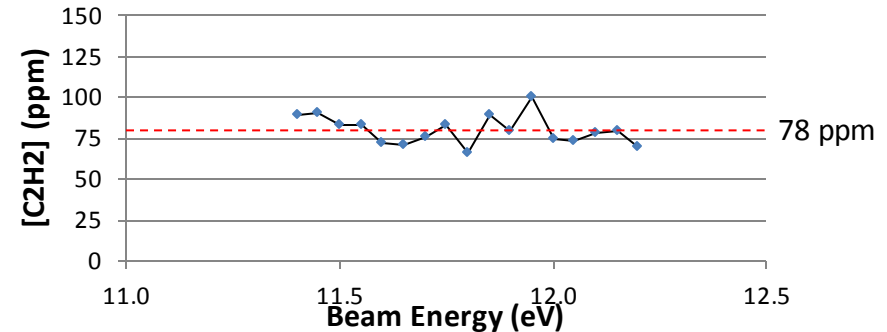
» Concentrations presented as a function of beam energy

- **High-O₂** NVO: -10 CAD_{NVO}
- ±25 ppm single energy uncertainty

» Signal conditioning may improve the measurement (e.g., wavelet denoising)

» VUV mass spec values ~20% lower than original GC measurements.

- Potential issues w/ apparatus sealing identified and will be accounted for.
- Results had good repeatability & indicated there was little impact from transport delay.



Follow-on experiments (FY15) will build on lessons learned from exploratory measurements.

Technical accomplishment 4: **Advanced Ignition Systems**

Detailed survey of advanced ignition challenges & opportunities

- » Solicited feedback on research approach/plans from **Chrysler**, **GM**, and **Ford** and identified common systems of interest.
- » Providing fundamental optical measurements of ignition phenomena to **Argonne** to in support of complementary modeling efforts in active LTGC lab.
- » Working w/ **USC** to perform a scoping study of their non-thermal transient plasma system.

Ignition system classes under consideration:

Thermal Plasmas/Lasers



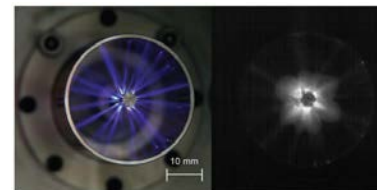
Pavel et al, Optics Express, 2011;19:9378-84.

Pre-Chamber



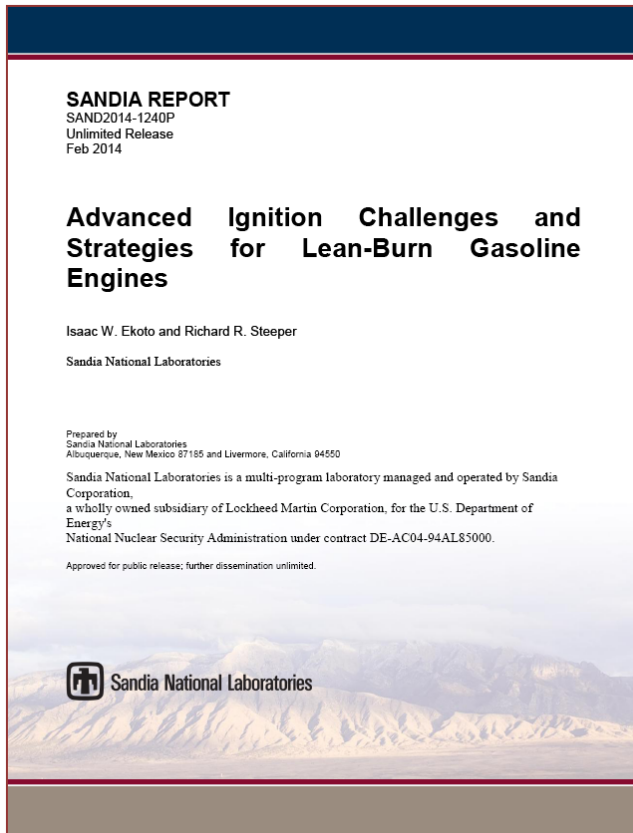
Attard, SAE Int J Engines, 2010;3:20-37.

Non-Equilibrium Plasmas



Singleton et al, J Phys D Appl Phys, 2011;44.

Initiated lab upgrades to a vacated engine lab to optimize for advanced ignition research.





Collaborations

»National Lab partners:

- Oak Ridge National Lab:
 - Joint NVO sampling experiments.
- Lawrence Livermore National Lab:
 - Assistance with NVO gas sample analysis via GC mass spec.
 - Ongoing development and support for chemical kinetics models.
- Argonne National Lab:
 - Experimental work in support of advanced ignition modeling.
- Lawrence Berkeley National Lab:
 - Experiments at the ALS to validate original GC measurements.

»University

- USC: Developed plans to use the Transient Plasma system for advanced ignition research.
- U. Minn.: Developed plans to explore **low-O₂** reforming research.

»Automotive OEM partners:

- GM Research: Extensive interactions w/ regular teleconferences that includes: 1) exchange of technical results, 2) hardware support, and active feedback on automotive LTGC research directions.
- Ford Research: Discussions and guidance on advanced ignition systems along with reactivity enhanced combustion via fuel reformation.
- Chrysler LLC: Discussions and guidance on advanced ignition systems.

»DOE Working Group partners:

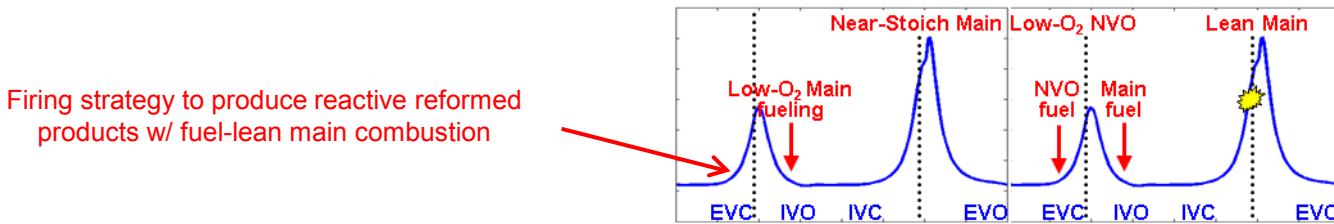
- Share research results at the DOE's Advanced Engine Combustion working group meetings.

»Remainder of FY14

- Continue post-processing ALS data to speciate low-O₂ and high-O₂ NVO engine samples.
 - Perform sensitivity studies for newly identified species & identify ways to improve future ALS experiment campaigns.
- Perform scoping studies for advanced ignition technologies:
 - Continue lab upgrades for advanced ignition work.
 - Perform high-speed imaging of ignition phenomena in support of Argonne modeling work.
 - Conduct a performance assessment of the USC transient plasma system in active lab.

»FY15

- Continue lab upgrades for advanced ignition research – target completion date: FY15Q4.
 - Upgrades include: installation of a spray guided head w/ improved optical access & higher possible peak pressures, a new high-pressure liquid fuel system, and updated data acquisition & gas delivery systems.
- Continue to work with Argonne to develop/validate RANS-based ignition modeling strategies.
 - Perform quantitative pre-ignition velocity measurements around ignition source.
- Establish long-term collaboration with USC testing the performance of their Transient Plasma system.
 - Perform exploratory measurements of low-temperature plasma radical species (e.g., OH, O, CO).
- Build on ORNL collaboration to explore low-O₂ operation to reform fuel for reactivity enhancement.
 - Identify interesting low-O₂ reforming operating points at ORNL & devise strategies to reproduce conditions at SNL.



- Conduct collaborative experiments & analysis w/ Prof. Will Northrup (U. Minn.) to identify favorable species produced from fuel reformation that impact main combustion – likely will involve future ALS experiments.



Summary

»Our work focuses on combustion control via NVO and advanced ignition systems, which enables efficient and clean automotive LTGC. Progress this year includes:

1. Sample experiments for low-load, high-O₂, NVO operation over a sweep of NVO injection timings.
 - Small saturated HCs increase rapidly as NVO SOI advances
 - Acetylene production accounts for 83% of the chemically induced main combustion phasing advancement, w/ hydrogen production responsible for the balance.
2. Replicated ORNL low-O₂ NVO experiments and obtained similar NVO product species results.
 - Initial results indicated bulk-gas reformation is the driving mechanism to produce highly reactive hydrocarbon species, which offers a new and potentially more controllable avenue for main combustion phasing control.
3. Conducted VUV mass spectrometry experiments at LBNL to clarify NVO sample measurements.
 - Experiments expected to validate earlier GC measurements & identify unique species that may impact main combustion.
 - Future projects possible for similar research.
4. Developed new research collaborations for advanced gasoline ignition.
 - Completed a detailed survey of advanced ignition challenges & opportunities for LTGC.
 - Initiated engine lab upgrades to create a dedicated platform for advanced ignition research.
 - Cultivated relationships with Argonne, USC, and the big 3 automotive OEMs.