Transportation Energy Center 8300

Automotive Low Temperature Gasoline Combustion Engine Research

Isaac Ekoto
Sandia National Laboratories

2015 DOE Vehicle Technologies Annual Merit Review
Arlington, VA
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Program Manager: Leo Breton & Gurpreet Singh
U.S. DOE Office of Vehicle Technologies

Project ID: ACE006

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Overview

Timeline

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

Barriers identified in VT Multi-Year Program Plan

- Lack of fundamental knowledge of advanced engine combustion regimes:
  - Investigate advanced combustion system concepts that enable high efficiencies and fuel injection strategies for the implementation of advanced combustion systems
  - Investigate mechanisms and strategies to reduce thermodynamic combustion losses
  - Research on combustion systems for advanced fuels

Budget

- Project funded by DOE/VT
- FY14 funding: $670k
- FY15 funding: $745K

Partners

- Project lead: Isaac Ekoto, Sandia National Laboratories
- Industry Partners:
  - GM, Ford, & Chrysler: technical guidance
  - 15 Industry partners in DOE Working Group.
  - Transient Plasma Systems Inc.
  - Advanced Technology Consultants, LLC
- University/National Lab Collaborators:
  - Oak Ridge National Lab: In-cylinder gas reformation
  - Lawrence Berkeley National Lab: Engine sample speciation
  - Argonne National Lab: Joint ignition experiments & modeling

Relevance & Objectives

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

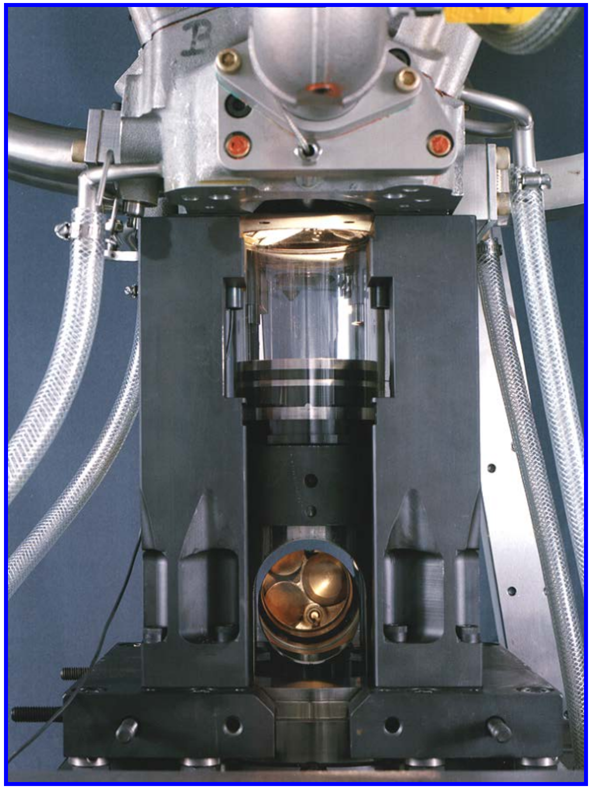
Specific FY15 objectives:

- Negative Valve Overlap (NVO): March 2014 – March 2015
  Re-compression of trapped exhaust gas via modified valve timings & a pilot fuel injection to provide subsequent main-cycle charge heating & reactivity enhancement
  - Identify NVO end-cycle reformate species using custom dump sampling and speciation by Gas Chromatography (GC) with varying NVO SOI, oxygen concentrations, and pilot fuel injection quantity
  - Analyze NVO end-cycle detailed sample speciation datasets acquired via photo-ionization mass spec and leverage these data to update in-house GC diagnostic calibrations
  - Clarify energy balance between oxidation and fuel pyrolysis driven NVO cycles
  - Evaluate opportunities for thermochemical recuperation – where retained exhaust sensible energy is converted into usable fuel energy – through kinetic modeling
  - Explore ethanol fuel effects on NVO reforming and oxidation processes – ***Stretch goal***
- Spark-Assisted Compression Ignition (SACI) : March 2015 – September 2015
  Flame propagation with controlled end-gas auto-ignition
  - Develop O-atom TALIF (two-photon laser-induced fluorescence) diagnostic to apply in optical engines
  - Perform particle image velocity measurements to support Argonne National Laboratory ignition modeling efforts
  - Demonstrate influence of non-equilibrium plasma igniters on low-load LTGC combustion stability – ***Stretch goal***

Sandia Automotive LTGC Optical Engine

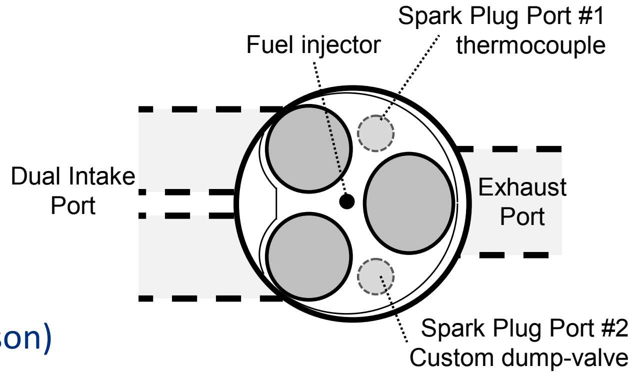
Engine Specifications

Head design	Pentroof
Displacement	0.63 liter
Bore	92 mm
Stroke	95.25 mm
Geometric compression ratio	11.5
Overhead cam shafts	Base and NVO
Valves	2 intake/1 exhaust
Direct injector	Vertical, central
Spark plugs	2 peripheral
Speed	2400 rpm
Peak cyl. press. (optical config.)	50 bar
Peak intake air pressure	1.5 bar abs.
Peak intake air temperature	220° C
Peak fuel pressure	150 bar



Diagnostics

High-speed imaging:	spray, ignition, combustion processes
Particle image velocimetry:	velocity fields
Laser-induced fluorescence:	fuel-air mixing, species specific detection
Diode laser absorption:	time-resolved species concentrations
Gas Chromatography:	dump-sample speciation



Engine suitable for low-load investigations

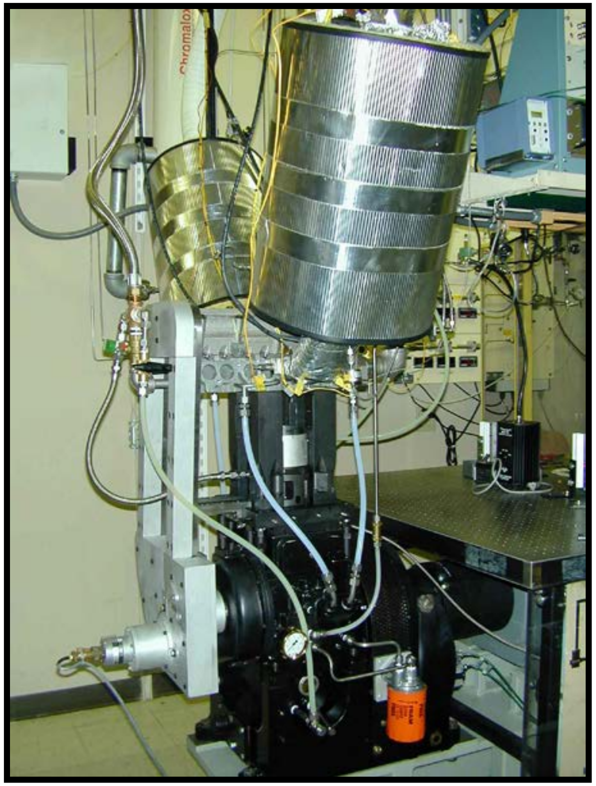
- ➢ Upgrades underway to enable cylinder pressures above 100 bar

Single component fuels to support sampling diagnostics

- ➢ Iso-octane, ethanol, (RD587 research gasoline for performance comparison)

Approach

- 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.
- Industry technology transfer of improved phenomenological understanding, technology demonstration, and developed models.



Approach - Milestones

Negative Valve Overlap

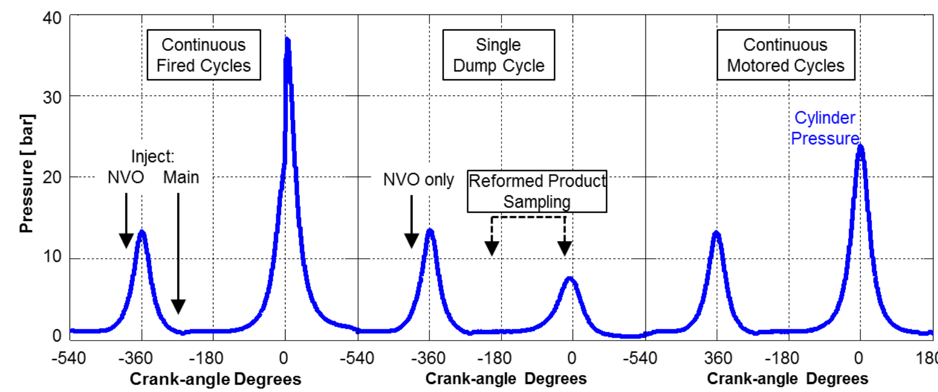
- Mar 2014 — Identify reformate species from oxygen deficient NVO periods via experimental engine dump sampling with speciation by Gas Chromatography
- Dec 2014 — Complete analysis of NVO engine samples from FY14 LBNL Advanced Light Source measurements
- Mar 2015 — Characterize NVO-cycle efficiency for oxidation and reformation dominated reactions through engine experiments and numerical analysis – ***FY15 Annual Milestone***
- Dec 2015 — Perform additional NVO sampling experiments to explore gasoline component fuel effects on NVO pyrolysis and oxidation processes

Spark-Assisted Compression Ignition

- June 2014 — Complete survey of advanced gasoline ignition challenges & opportunities
- June 2015 — Perform exploratory measurements of O-atom laser induced fluorescence from a plasma assisted laminar reference flame
- Sep 2015 — Provide in situ mixing and flow-field data prior to and during the ignition event to Argonne to support complementary multi-dimensional modeling
- Mar 2016 — Demonstrate influence of non-equilibrium plasma igniters on low-load LTGC combustion stability – ***FY16 Annual Milestone***

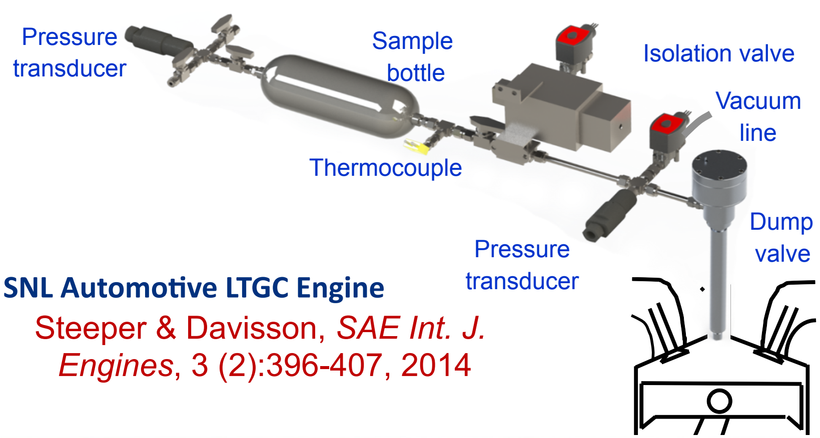
Accomplishment: Photo-ionization mass spectroscopy of NVO cycle engine samples

- Dump-valve
  - Full-cylinder gas sampling
  - Heated sample bottle (1000 ml, 90°C)
- Custom dump sampling event
  - Air-op solenoid isolation valves to limit impact of dump-valve leakage
  - ~7 engine cycles to fill bottle
- SNL flame sampling apparatus
  - Photo-ionization by a continuous & tunable soft X-ray beam (7.8 to 17 eV)
  - Speciation by time-of-flight mass spec
    - Isomer identification possible



Lawrence Berkeley Advanced Light Source

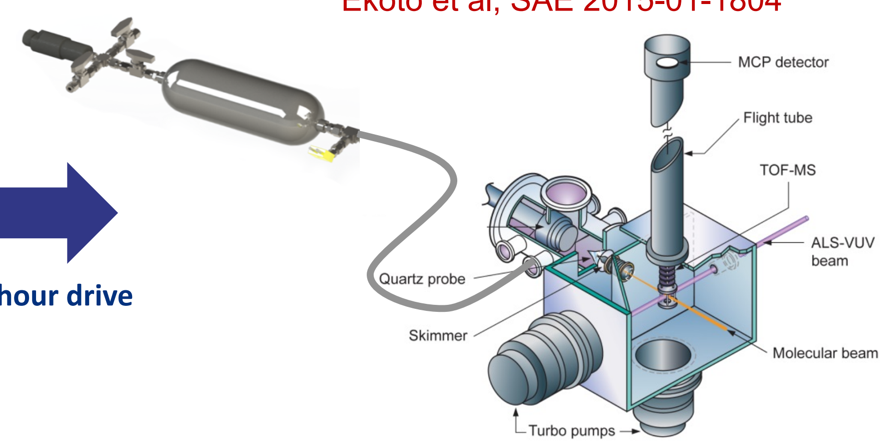
Ekoto et al, SAE 2015-01-1804



SNL Automotive LTGC Engine

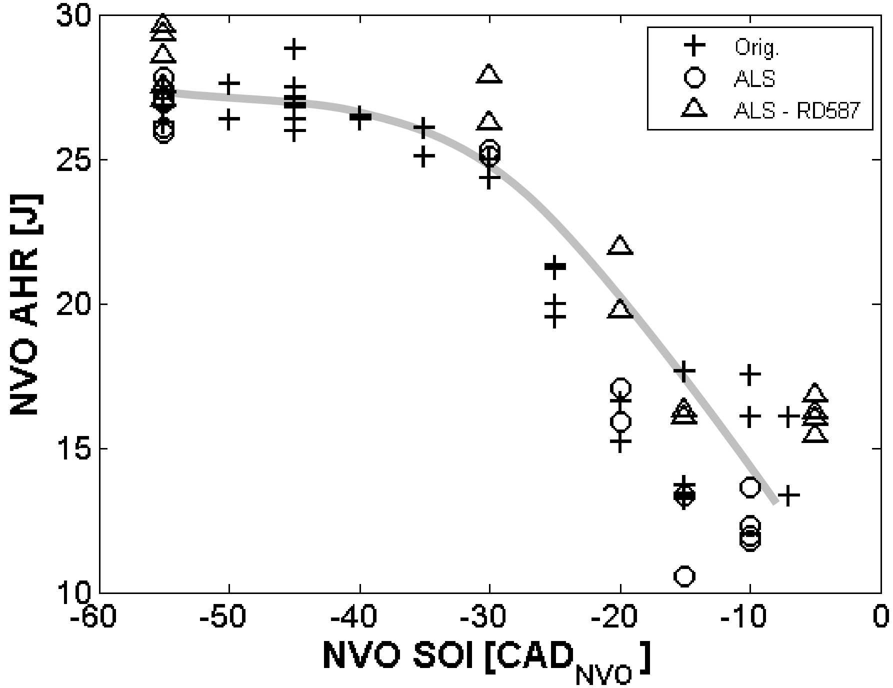
Steeper & Davisson, *SAE Int. J. Engines*, 3 (2):396-407, 2014

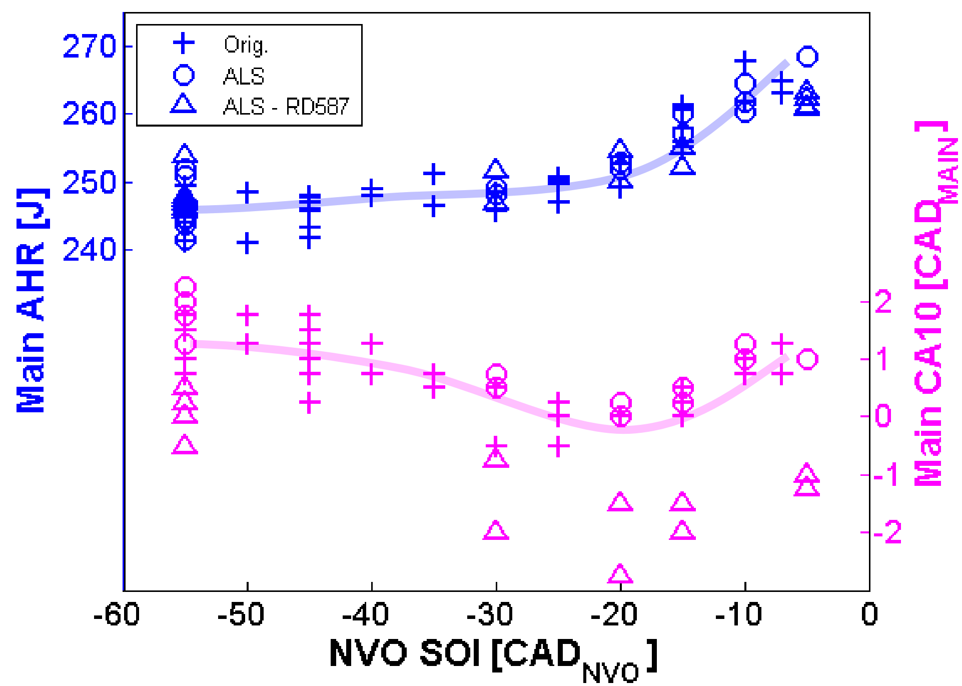
1 hour drive



Accomplishment: Photo-ionization mass spectroscopy of NVO cycle engine samples – cont.

- NVO and main heat release characteristics consistent with previous results



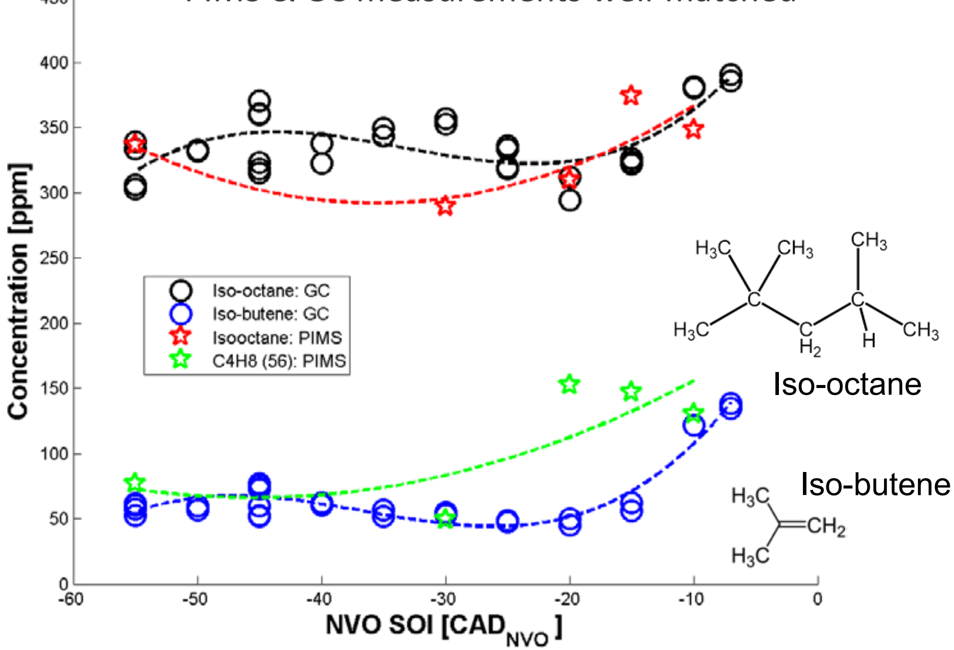


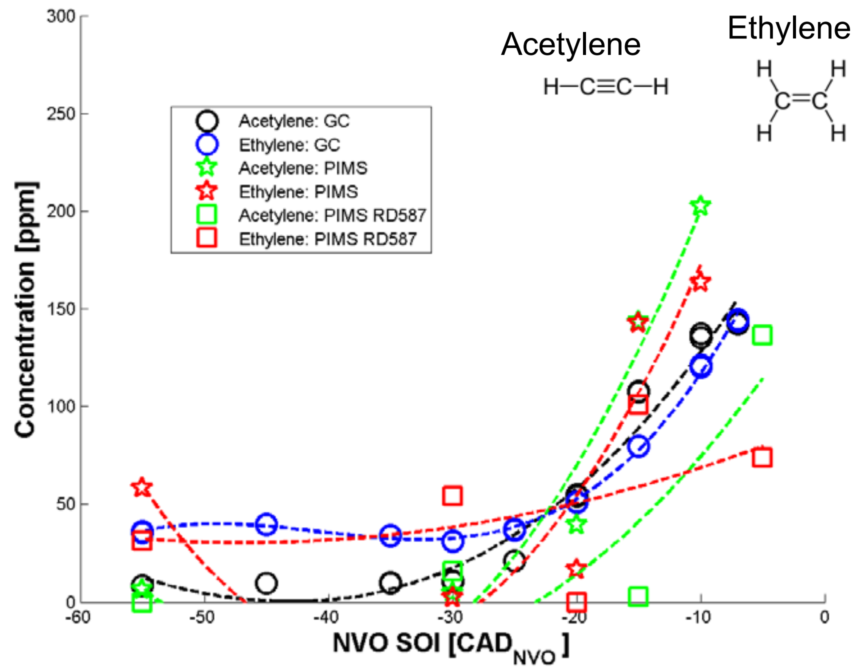
- RD 587 fueling
  - Slightly higher NVO period heat release (~1-2 J)
  - Slightly advanced main combustion phasing (~2 CAD).
  - Main heat release well matched

<u>Operating conditions:</u>
- NVO O_2: 7%
- T_{intake}: 120°C; T_{EVC}: 404°C
- Split inject: 1.2 + 8.4 mg

Accomplishment: Photo-ionization mass spectroscopy of NVO cycle engine samples – cont.

- Custom data reduction methods developed to make diagnostic quantitative
- Large HC Invariant across NVO SOI sweep
  Steeper & Davisson, *SAE Int. J. Engines*, 3 (2):396-407, 2014
  – PIMS & GC measurements well-matched
- Acetylene shown to impact main-cycle reactivity
  Puranam & Steeper, *SAE Int J Engines* 5(4):1551-60, 2012.





- GC Iso-butene is the sum total of all isomers
  – PIMS enables isomer concentration breakdown (not shown to preserve clarity)
- Acetylene/Ethylene results well-matched
  – RD587 fueling measurements also well-matched (larger species could not be resolved)
- Additional quantitative information for isomers, oxygenates, and aromatics obtained
  – Used to update palate of GC calibration gases

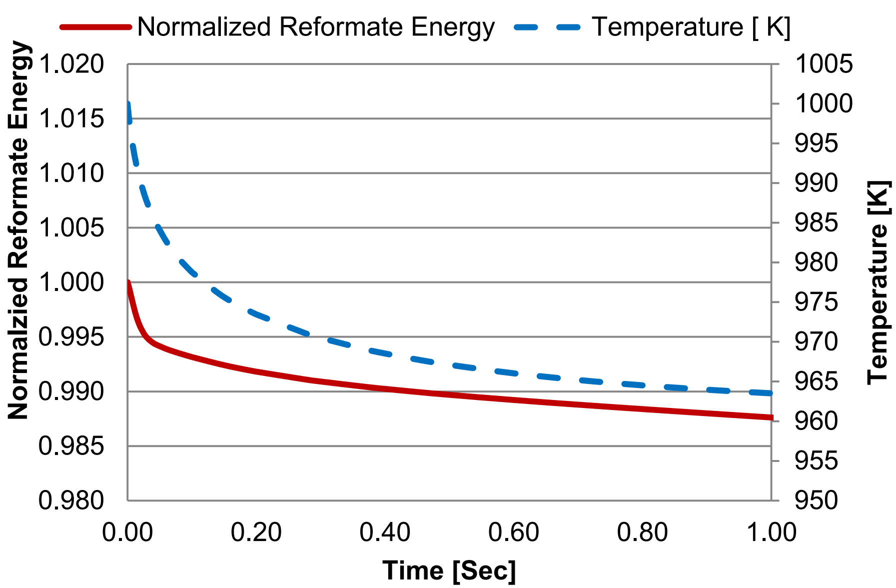
Ekoto et al, SAE 2015-01-1804, PFL Meeting, Kyoto

Accomplishment: Numerical evaluation of thermochemical recuperation

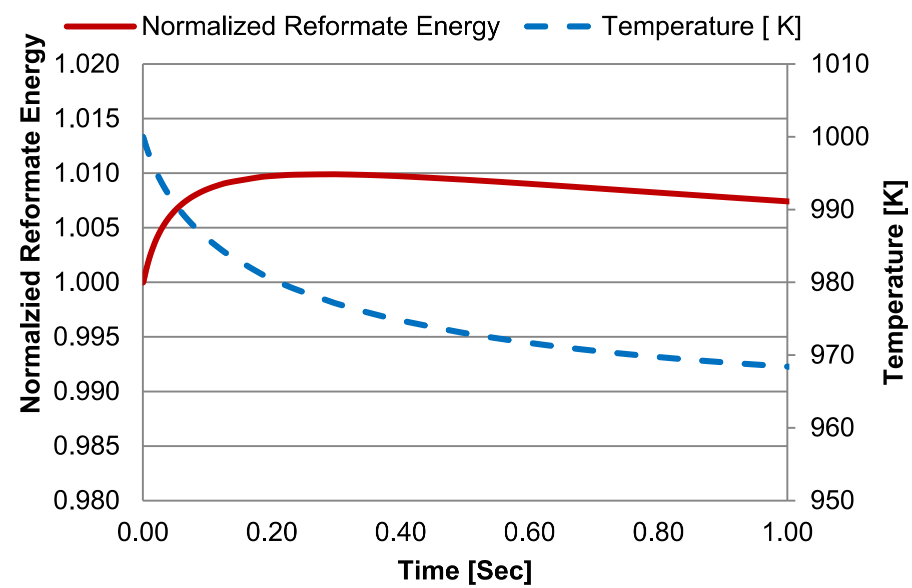
- Sensible exhaust energy converted to usable fuel energy through pilot fuel reformation
  Szybist JP, et al, *Energ Fuel*, 26 (5):2798-810, 2012
  - Fuel dependent process

Constant pressure homogeneous reactor simulations
Initial Temp: 1000 K
Pressure: 8 bar
Non-fuel components: 80% N_2, 10% H_2O, 10% CO_2
Fixed fuel energy amount representative of NVO

Iso-Octane Reformate



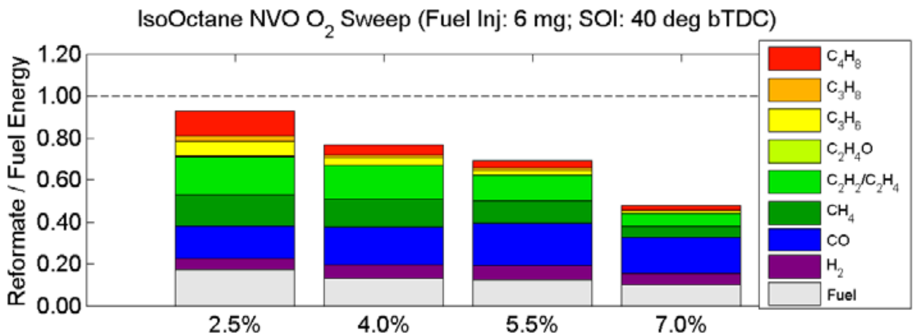
Ethanol Reformate



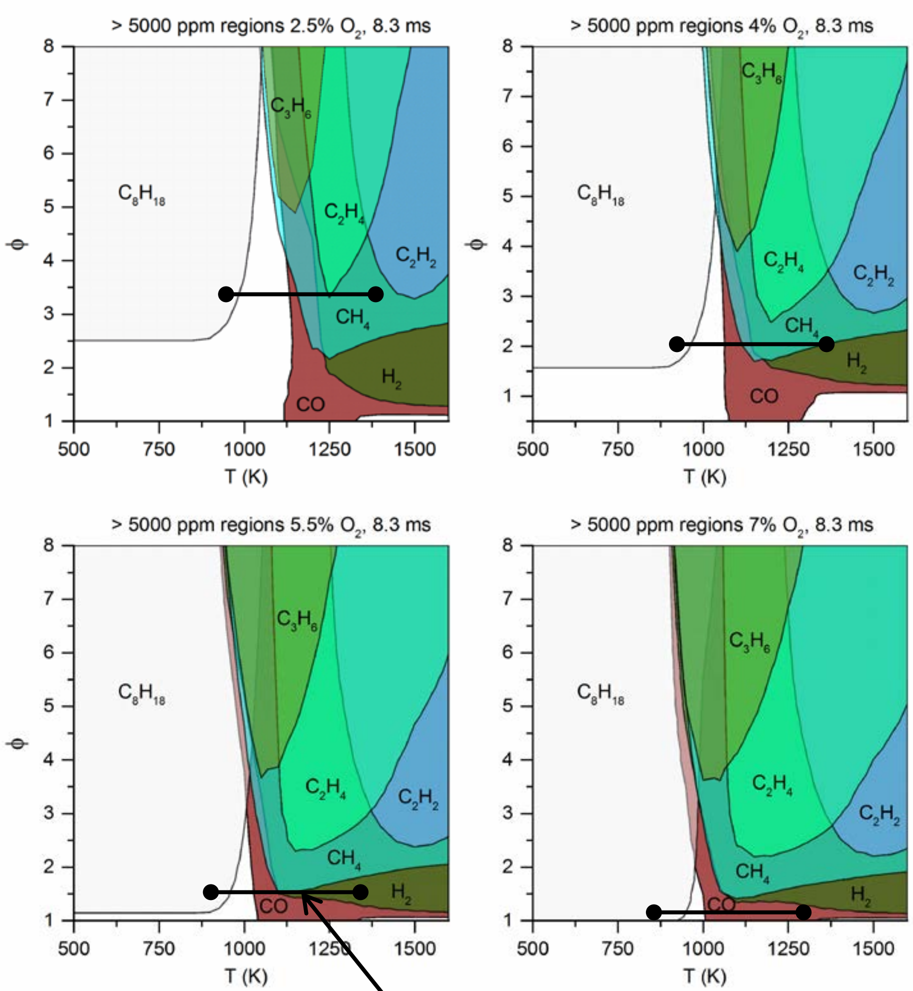
- Up to 1% additional fuel energy from ethanol reformate
- Process is very slow relative to NVO period residence times (~20 ms @ 1200 RPM)

Accomplishment: Efficiency analysis of NVO cycle oxidation & reforming

- Fixed SOI & fueling w/ variable NVO O_2
  - Invariant CO, H_2, & parent iso-octane
  - Lower fuel energy recovered w/ higher O_2 due to lower intermediate HC yields



Peterson et al, SAE World Congress, 2015-01-0818

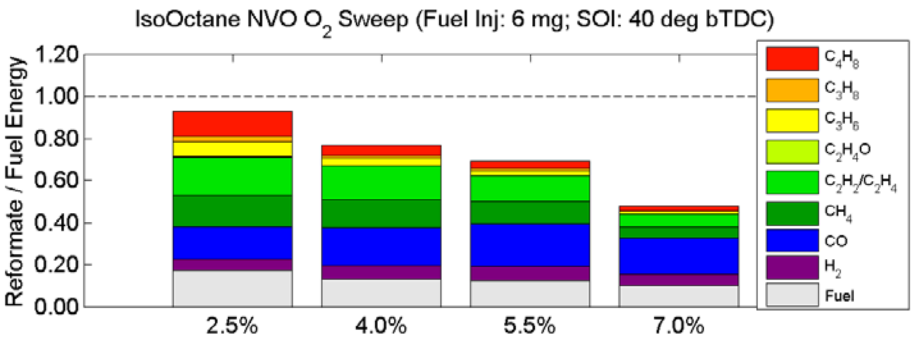


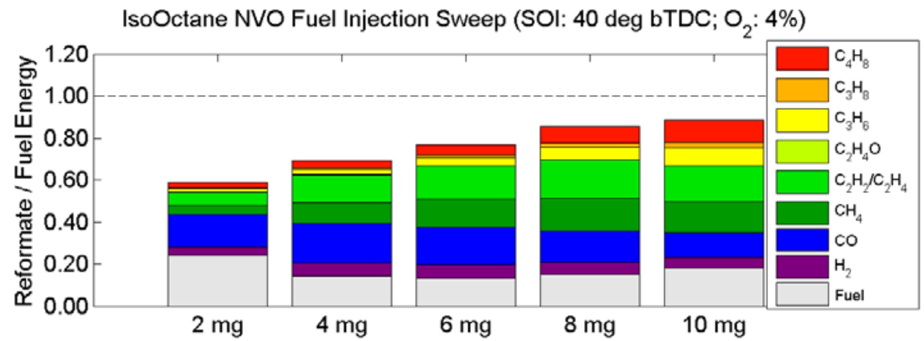
Representative bulk-gas temperature range

- Homogeneous reactor simulations
  - Isobaric (8 bar) w/ energy conserved
  - Representative 8.3 ms residence time
  - Higher NVO O_2 $\rightarrow$ lower ϕ
- Lower NVO O_2 $\rightarrow$ higher ϕ
  - Mixtures shift away from O_2 limited HC formation islands

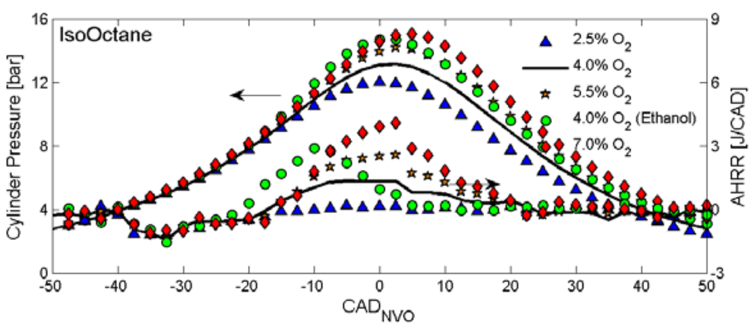
Accomplishment: Efficiency analysis of NVO cycle oxidation & reforming – cont.

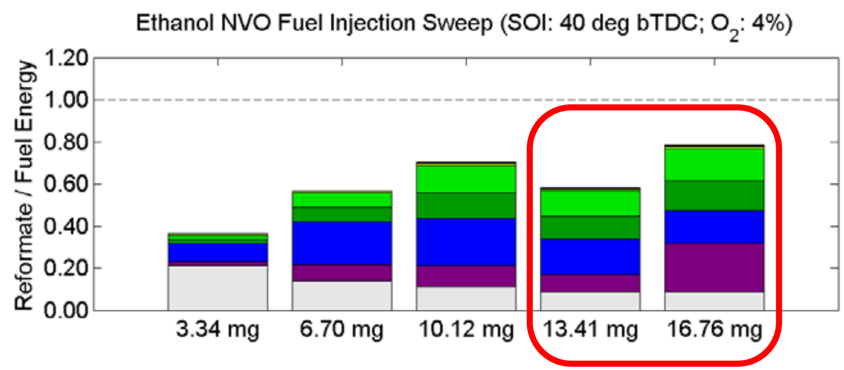
- Fueling rate sweeps (4% O_2, 6 mg inj) with equivalent ethanol conditions:
  - Ethanol fuel energy injected adjusted to match corresponding iso-octane condition
  - Lower fuel energy yield due to increased heat release
  - **Fuel Injector problems for 2 highest fueling rates**





Peterson et al, SAE World Congress, 2015-01-0818





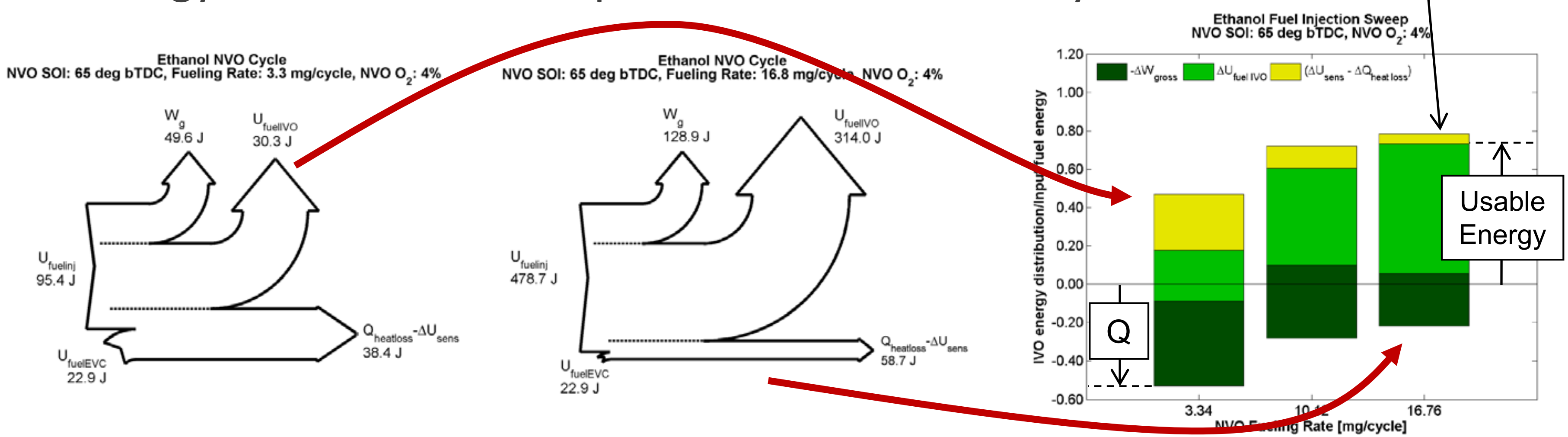
- Steady increase in heat release with O_2 concentration
  - Ethanol fueled conditions had more heat release than equivalent IO fueled conditions

Accomplishment: Efficiency analysis of NVO cycle oxidation & reforming – cont.

- Energy Balance Calculations:
  - **Fuel energy:** Injected fuel energy + Energy from GC measured species
    - Sampling w/o NVO fueling used to estimate fuel energy into the NVO period
      Szybist JP, Chakravathy K, Daw CS, *Energ Fuel*, 26 (5):2798-810, 2012
  - **Sensible energy:** GC measurements & thermodynamic properties
    - Only change in closed-cycle NVO sensible energy considered
      Fitzgerald RP, et al, *SAE Int. J. Engines*, 3 (1):124-41, 2010
  - **Heat Loss:** Modified Woschni correlation from measured pressure
      Chang J, et al, SAE Paper 2004-01-2996
  - **Gross Work:** Integrated heat release – heat loss

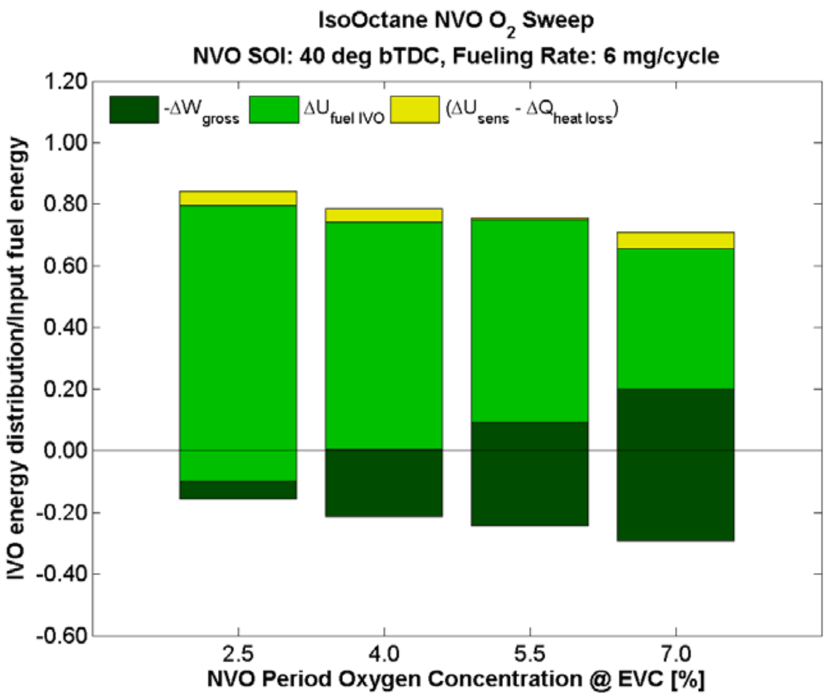
Positive → Charge heating
Negative → Thermochemical recuperation

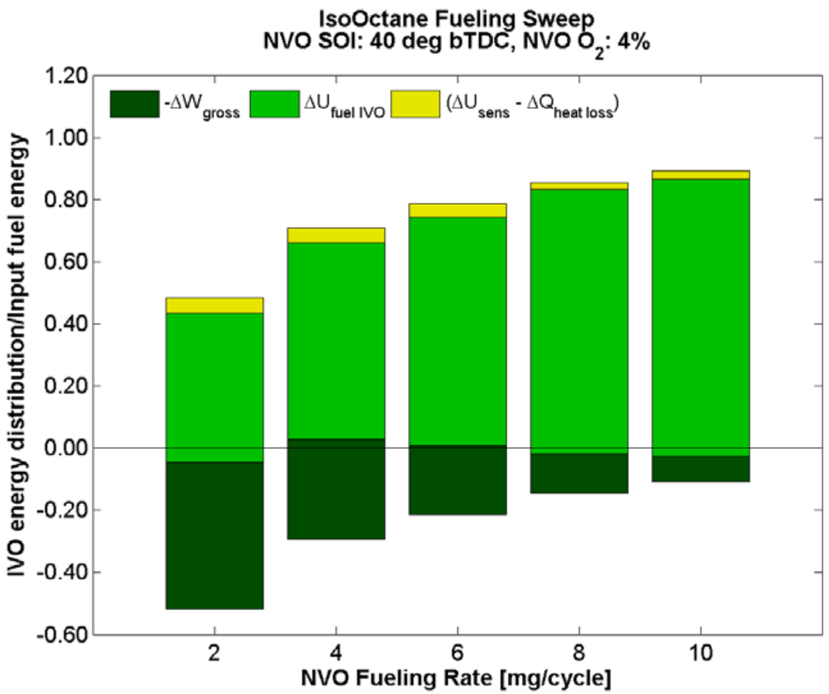
- Energy balance can be expressed in different ways



Accomplishment: Efficiency analysis of NVO cycle oxidation & reforming – cont.

- Measures that ↑ϕ (e.g., ↓ NVO O_2 or ↑ fueling rate) improve energy recovery
- Gross work largely balanced by heat loss due to inefficient heat release from:
  - Slow reaction rates, small compression ratios and high specific heat ratios
- No thermochemical recuperation for iso-octane achieved – confirms simulation results





Ekoto, IW, Peterson, BR, Szybist, JP, Northrop, W 15ICENA-0124

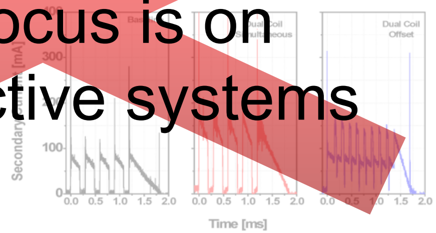
- Better opportunities for energy recovery should exist with ethanol fueling

Accomplishment: Exploratory Spark-Assisted Compression ignition experiments

~~Enhanced Induction Spark~~

- ~~Multi-strike~~
- ~~Multi-spark~~
- ~~Continuous Discharge (e.g., DEIS or DCO)~~

DOE focus is on non-inductive systems

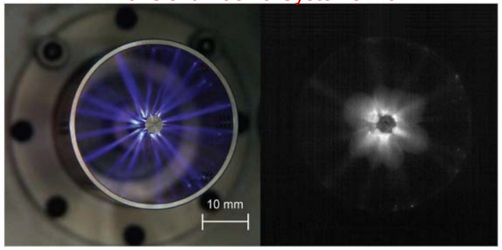


Alger et al, SAE Int J Engines, 2011;4:677-92.

Non-Equilibrium Plasma

- Microwave Assist
- Plasma initiated (RF or nanosecond discharge)

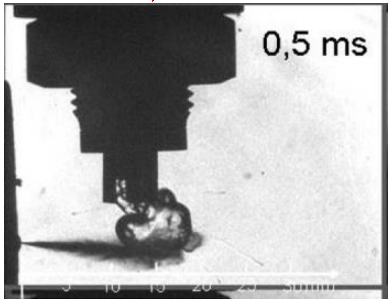
Transient Plasma Systems Inc.



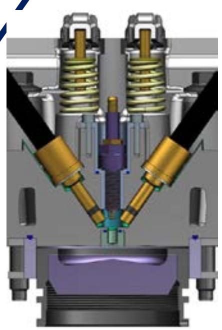
Thermal Plasma

- Plasma Jet
- Railplug

Knite inc. ,DE-SC001944



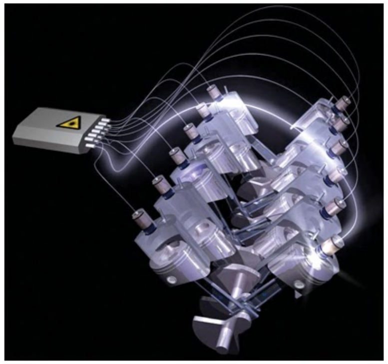
Turbulent Jet Ignition



Michigan State University, NSF/DOE Partnership Grant, 1258581

Laser Ignition

- Non-resonant breakdown
- Resonant breakdown
- Light activated particle ignition



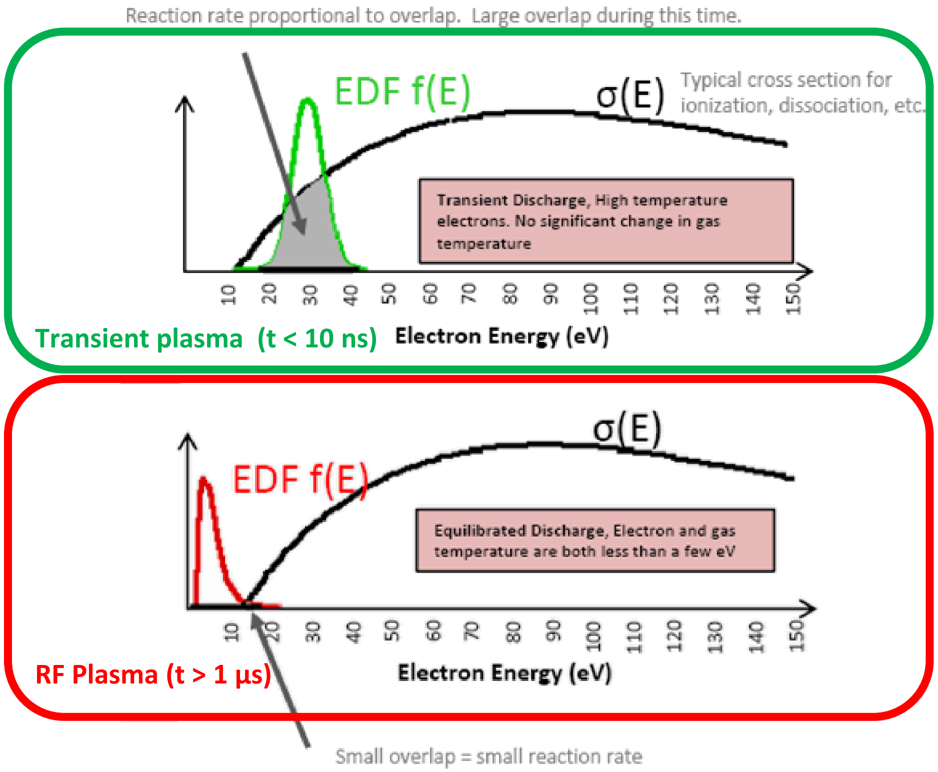
Princeton Optronics DOE SBIR: 212124

- Promising advanced ignition systems for SACI applications identified

Accomplishment: Exploratory Spark-Assisted Compression ignition experiments

Reactive radical formation rate $\propto \int f(E)\sigma(E)dE$

- σ: Ionization cross-section
- f: Electron distribution function
- E: Electron energy



Pulse generator

Transient Plasma 40 kV Solid State Pulse Generator	
Max rep rate (burst mode)	10 kHz
Max burst pulse train	20
Max system rep rate	100 Hz
Max pulse energy	Load Dependent (~40 mJ)
Pulse width	12 ns FWHM (fixed)

- **Goal: Operate below the electrode breakdown threshold to achieve radical augmented ignition**
- Experiments underway to explore influence of pulser settings & electrode geometry on engine performance
  - Future collaboration plans w/ boosted LTGC work (John Dec)

Accomplishments - Overview

Negative Valve Overlap

- Completed analysis of NVO end-cycle detailed sample speciation data acquired at the LBNL Advanced Light Source by photo-ionization mass spectroscopy
  - Joint project that leveraged Sandia's BES Combustion Chemistry capabilities
  - Updated in-house GC diagnostic calibrations based on results
  - Performed new ALS experiments
- Analyzed the efficiency tradeoff between oxidation and reforming dominated NVO-cycles
  - Performed NEW sampling experiments with the engine operated under a range of NVO SOI, cycle oxygen concentrations, and pilot fuel injection quantities
  - Numerically evaluated opportunities for thermochemical recuperation through kinetic modeling
  - Calculated energy balance (gross work, heat loss, fuel energy recovered, change in sensible energy) using detailed sampling data & custom data reduction codes
  - Evaluated NVO cycle efficiency for ethanol fueling

Spark-Assisted Compression Ignition

- Exploratory O-atom laser induced fluorescence
  - Purchased necessary capitol equipment (high-voltage nanosecond discharge pulser, ICCD camera with good quantum efficiency in red) to go along with an in-house, tunable, high-power laser
  - Setting up for exploratory experiments in May/June timeframe

Reviewer Response

R1: Was the source of increased acetylene from piston wall wetting?

Response: The reviewer is referred to the FY12 AMR presentation where optical evidence of fuel film impingement with late injection was definitively observed for high O_2 environments. For low O_2 NVO, acetylene was instead attributed to bulk fuel reformation; confirmed in this year's experiments.

R2: It was not clear exactly what kind of combustion concept was going to be investigated. It was also not clear exactly how the ignition studies were going to relate to the combustion concept.

Response: We are focused on LTGC-like operating conditions that feature elevated compression ratios, heavy dilution, and compression induced auto-ignition. Our particular focus is at low-loads where combustion stability is challenging. As such, our ignition work focuses on systems that can improve this combustion stability while maintaining good efficiency and emissions performance.

R3: The reviewer would like to see the NVO work translated into a "controls" approach to ensure good combustion, efficiency, & emissions over a range of speeds, loads, & environment conditions.

Response: This is likewise our goal. As such, we focused on NVO period energy balance over a range of environment conditions and fueling rates. We have augmented these data with kinetic modeling to better understand important physical processes, which will inform future efforts at full-cycle analysis.

R4: The work needs to demonstrate the effects of oxygenated species (e.g., in Fuels for Advanced Combustion Engines [FACE] fuels) on the NVO mechanisms being examined.

Response: Initial work into ethanol fuel effects was started this FY. We have additional FY16 plans to continue this work and examine other relevant gasoline fuel components and surrogates.

Collaborations

- National Lab
  - Oak Ridge National Lab: Joint NVO sampling experiments and analysis.
  - Argonne National Lab: Complementary modeling support for advanced ignition experiments,
  - Lawrence Berkeley National Lab: Detailed NVO sample speciation at the ALS,
  - Sandia BES program: Joint proposal developed to explore physics of low-temperature plasmas.
- University
  - USC: Ongoing collaborative research on low-temperature plasma ignition.
  - U. Minn.: 2 month Sandia sabbatical by Prof. Will Northrop to explore NVO cycle efficiency.
  - U. Edinburgh: Ongoing analysis of reforming chemistry during NVO.
- Automotive OEM
  - GM Research: Extensive interactions w/ regular teleconferences that includes: 1) technical results exchange, 2) hardware support, & 3) 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.
- Small business
  - Transient Plasma Systems Inc.: Supplied Sanida with a custom high-voltage pulse generator needed for low-temperature plasma ignition studies, along with ongoing support.
  - Advanced Technology Consultants LLC: Plans developed to investigate a novel light activated ignition system of seeded carbon nanotubes within the Sandia automotive LTGC engine.
- DOE Working Group
  - Share research results at the DOE's Advanced Engine Combustion working group meetings.

Future Work:

- Remainder of FY14
  - Perform exploratory O-atom two-photon laser induced fluorescence (TALIF)
    - Integrate high-voltage nanosecond pulser w/ custom electrodes to generate atomic O
    - Image atomic O via TALIF using an in-house, tunable, high-power, laser source & a new ICCD camera with good near-IR sensitivity
  - PIV datasets to support of Argonne National Laboratory ignition modeling work
- FY15 Future work
  - Evaluate NVO reformation and oxidation processes for gasoline FACE components
  - Evaluate the impact of low-temperature plasma igniter electrode geometry on dilution limits for spark-assisted compression ignition (SACI)
  - Develop O-atom TALIF diagnostic so that it can be applied in an optical engine
    - Develop signal model to account for TALIF photo-physics
    - Perform custom alterations to optical engine (e.g., high-purity windows)
  - Identify low-load LTGC operating points where performance metrics (efficiency, noise, emissions) are poor, but significantly improve with the use of NVO or SACI.
    - Analyze the relative benefit of each technology

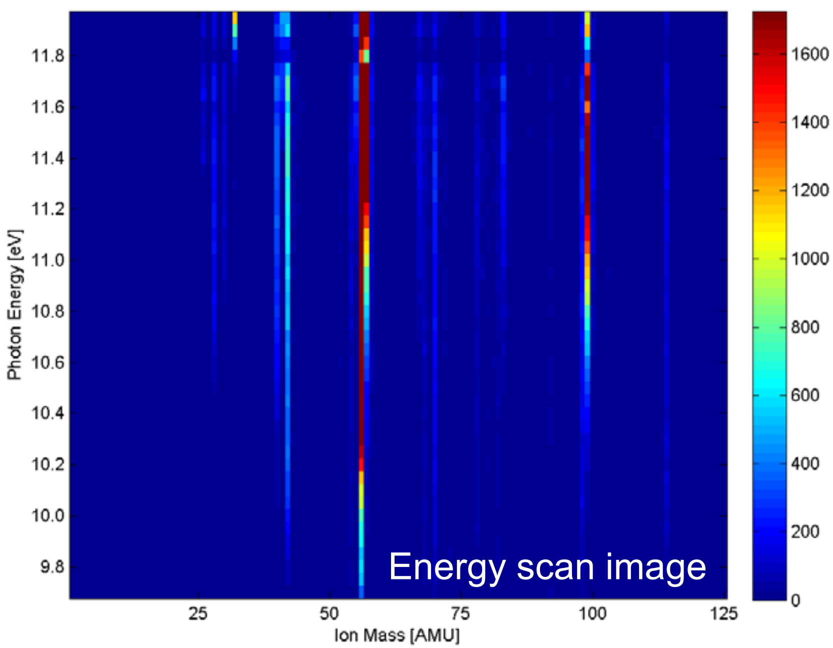
Technical Backup Slides

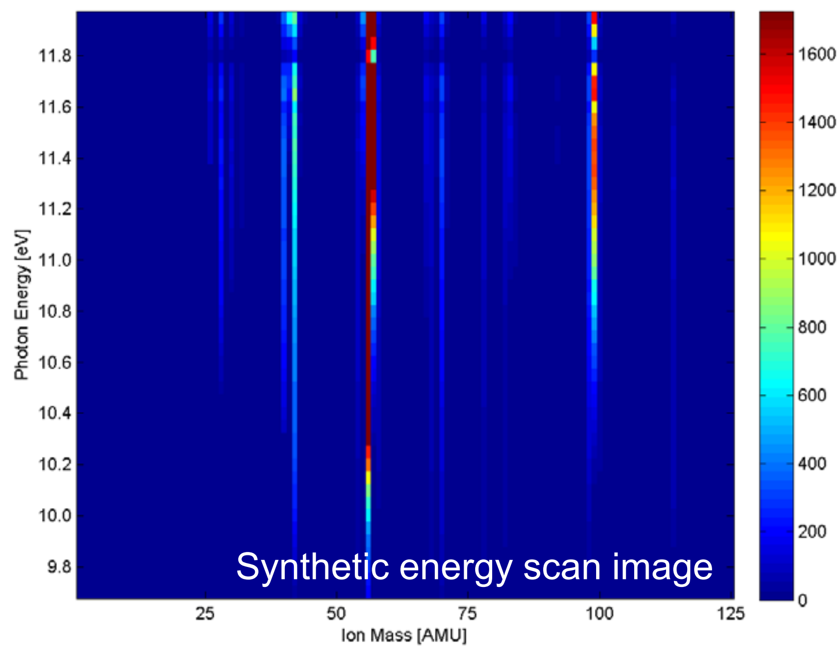
Technical backup slide: PIMS signal modeling

- Measured signal, *S*, is the total contribution from each species, *i*, at energy, *E*.
  - *X*: species concentration
  - *σ*: photoionization cross-section (PICS)
  - *D*: mass discrimination factor
  - Φ: photon flux
  - PD_{eff}: photodetector efficiency
  - SW: number of sweeps
  - C: calibration constant

Iteratively adjusted to best fit data

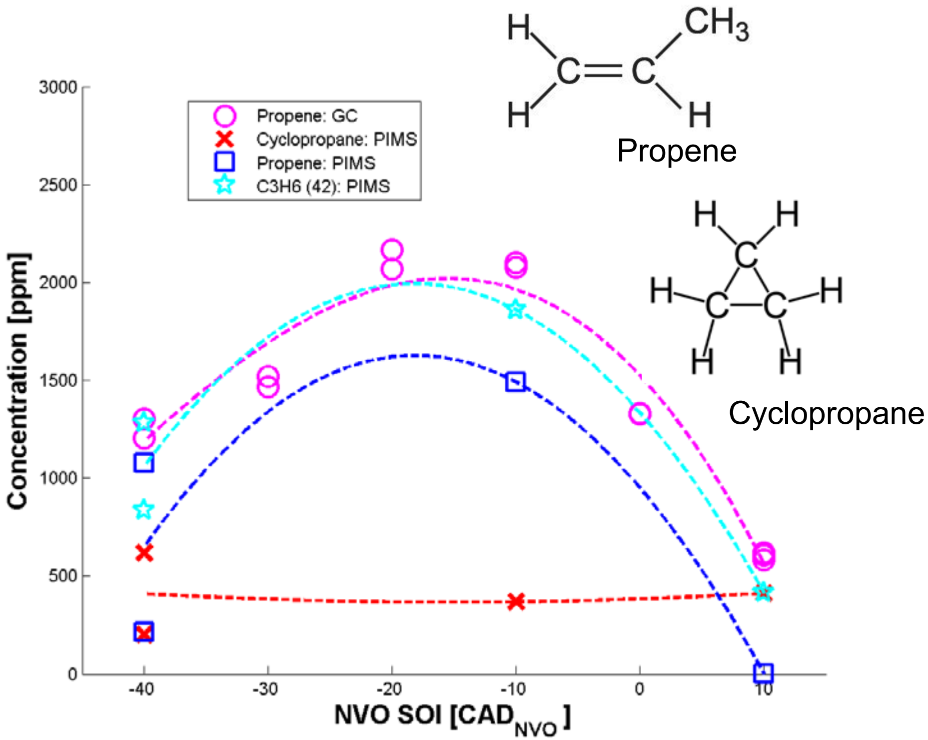
$$S_i(E) = \chi_i \cdot \sigma_i(E) \cdot D_i \cdot \Phi(E) \cdot PD_{eff}(E) \cdot SW(E) \cdot C(E)$$

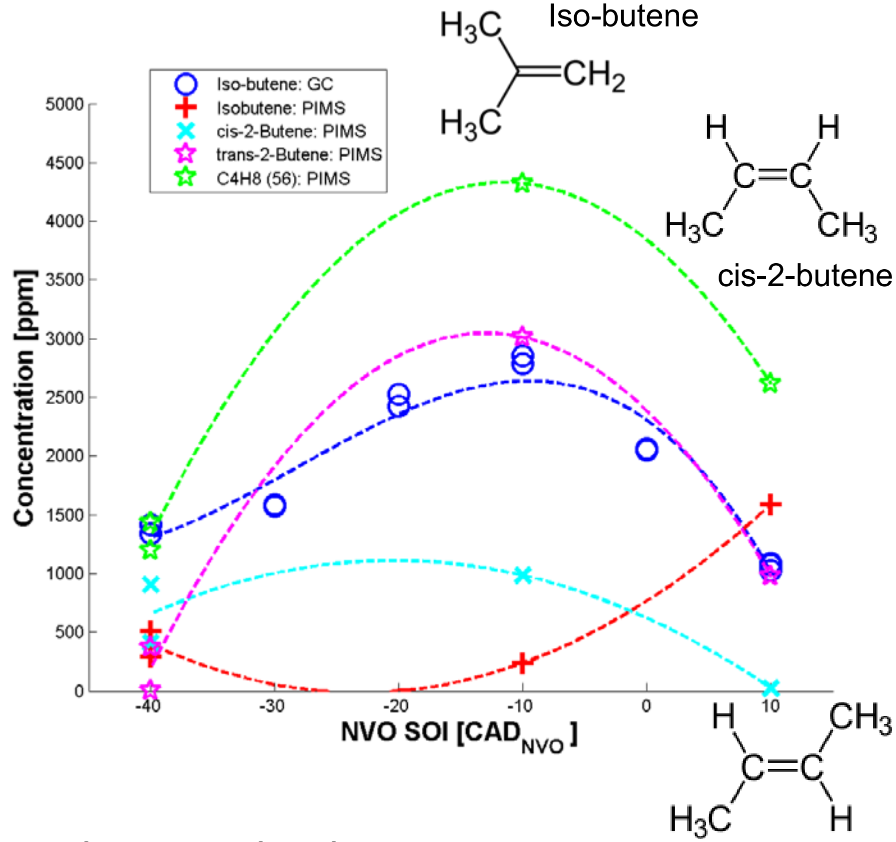




Technical backup slide: Detailed NVO sample speciation results by PIMS

- C3H6: Baseline cyclopropane with varying contributions from propene



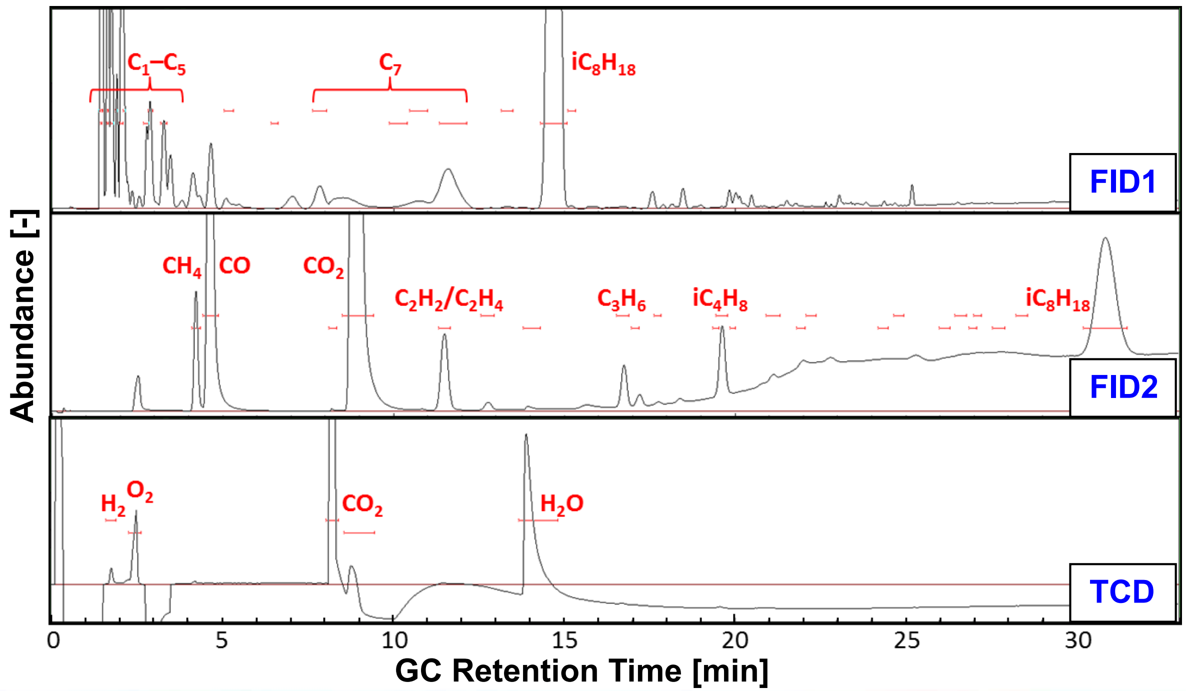


trans-2-butene

- C4H8: Consistent trends for most isomers but total values
  - GC sensitivity likely differs for each species

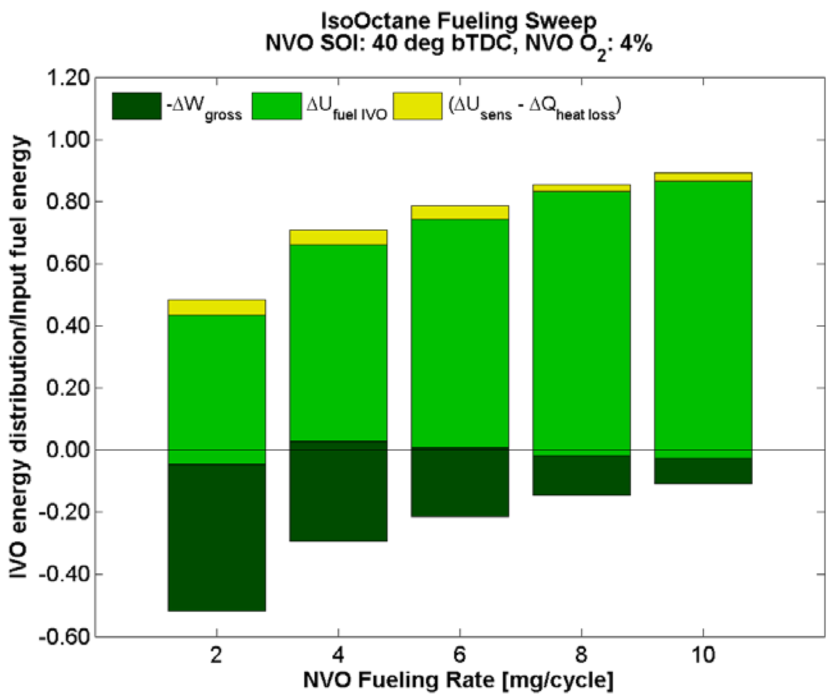
Technical backup slide: NVO sample speciation by Gas Chromatography

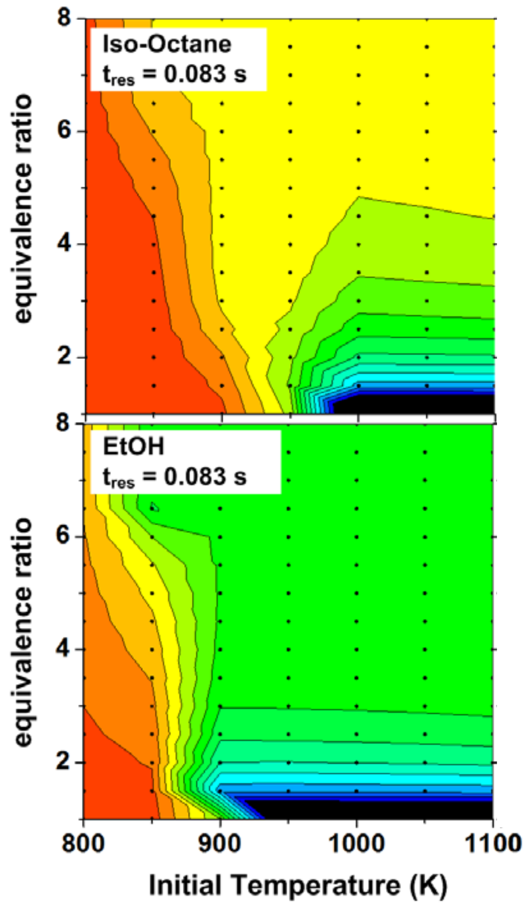
- GC houses 3 detectors: 2 flame ionization (FID) and 1 thermoconductivity (TCD).
  - FID1: Quantifies intermediate and large hydrocarbons
  - FID2: Uses a different column to spread out C_1 to C_3 hydrocarbons
    - . Includes a methanizer to detect CO & CO_2.
  - TCD: hydrogen, oxygen, and water
  - Repeatability is better than ±10% for most species of interest
  - ***Signal observed from several unknown species***



Technical backup slide: NVO energy recovery experiments vs. simulations

4% O_2





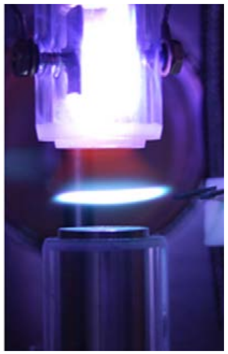
- Simulation energy recovery consistent with experiments

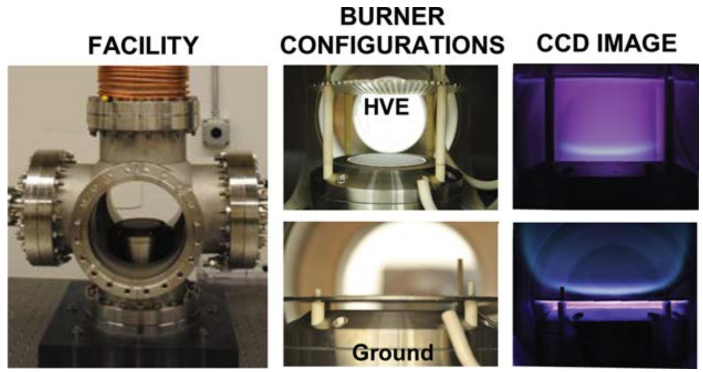
Ekoto, IW, Peterson, BR, Szybist, JP, Northrop, W 15ICENA-0124

Technical backup slide: Proposal for fundamental low-temperature plasma research

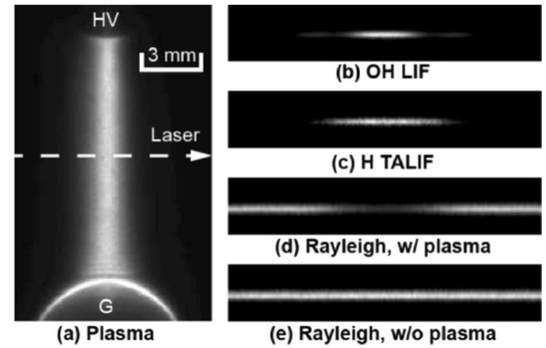
Recent experiments in the literature:

Low-pressure flames:





Low-pressure premixed 1D flame

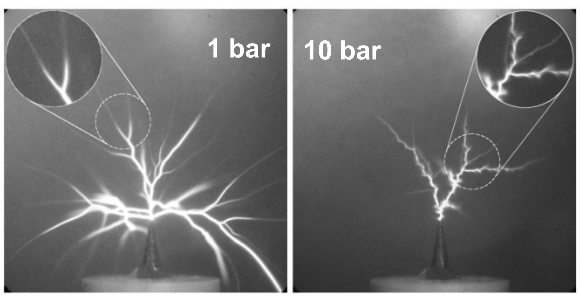


Sun et al, *P Combust Inst*, 2011;33:3211-8
Sun et al, *Combust Flame*, 2012;159:221-9

Li et al, *Combust Sci Technol*, 2013;185:990-8

Yin et al, *P combust Inst*, 2015;34:3455-62

High-pressure chamber



F. Auzas, Thesis, Université Paris Sud–XI, 2008

High-pressure chamber

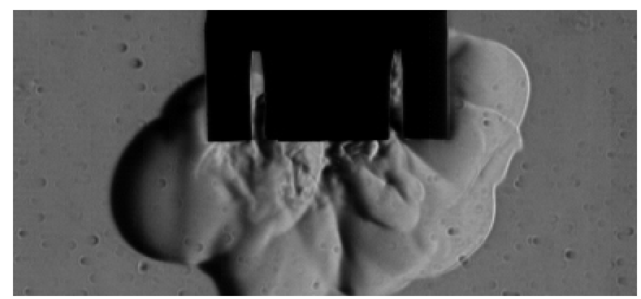


Image courtesy of Dan Singleton, Transient Plasma Systems Inc., 2015

- Experiments w/ Sandia BES program to characterize non-equilibrium plasmas
- Complementary engine experiments with *in situ* diagnostics