TRANSPORTATION ENERGY CENTER 8300

Gasoline Combustion Fundamentals

Isaac Ekoto (PI), Benjamin Wolk
Sandia National Laboratories

2016 DOE Vehicle Technologies Annual Merit Review
Washington, DC
June 8, 2016 – 10:00 a.m.

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

- Insufficient knowledge base for advanced LTC or mixed-mode combustion systems over full load range
- Models needed for fundamental engine combustion and in-cylinder emissions formation processes
- Lack of effective engine control for advanced lean-burn direct injection gasoline engine technology

Budget

- Project funded by DOE/VT
- FY15 funding: $745K
- FY16 funding: $675K

Partners

- Project lead: Isaac Ekoto, Sandia National Laboratories
- Industry/Small Business Partners:
  - GM, Ford, & Chrysler: technical guidance
  - 15 Industry partners in DOE Working Group.
  - Transient Plasma Systems Inc.
- 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
  - U. Minnesota: Engine sample speciation
  - Michigan State University: Turbulent jet ignition

Relevance & Objectives

Project objective: Expand fundamental understanding of fluid-flow, thermodynamics, and combustion processes needed to achieve clean and fuel-efficient gasoline engines.

FY16 objectives:

- Clarify impact of reformate addition from the negative valve overlap period (NVO) on low-temperature gasoline combustion (LTGC) auto-ignition
  - Characterize constituents of in-cylinder generated reformate for common gasoline fuel components
  - Identify dominant constituents that influence auto-ignition chemistry via single-zone kinetic modeling
  - Examine influence of fuel reformate addition on main-period combustion behavior

Impact: Provides a basic understanding of the thermodynamic & chemical details of improved main-cycle reactivity when main fueling is blended w/ fuel reformate from a NVO period

Benefit: Enables improved low-load control for LTGC & tests model predictive capabilities

- Spark calorimetry w/ *in situ* radical measurement of low-temperature plasma (LTP) and nanosecond pulse discharge (NPD) ignition
  - Measure electrical-to-thermal efficiency for SI inductive spark, LTP, and NPD ignition
  - Quantify O radical formation as a function of ambient pressure for LTP ignition
  - Evaluate influence of LTP and NPD ignition in newly built single-cylinder research engine

Impact: Unique capability used to investigate impact of electrode position/geometry on high-pressure plasma physics and chemistry in fuel-air mixtures

Benefit: Advances LTP and NPD igniter development for dilute high-efficiency gasoline engines

Milestones

Date	Milestones	Status
December 2015	<u>Milestone:</u> Identify important reformate species from FY15 photoionization mass spec (PIMS) measurements that influence auto-ignition chemistry.	Complete
March 2016	<u>Milestone:</u> Evaluate fuel reformate composition and influence on main-period fuel reactivity for gasoline FACE components.	Complete
June 2016	<u>Milestone:</u> Quantitatively measure atomic oxygen generated by low-temperature plasmas via two-photon absorption laser induced fluorescence (O TALIF).	Complete
September 2016	<u>FY16 Annual Milestone:</u> Evaluate dilute combustion stability limits for low-temperature plasma ignition with different electrode configurations.	On track

Approach: Clarify impact of NVO generated reformate on LTGC auto-ignition

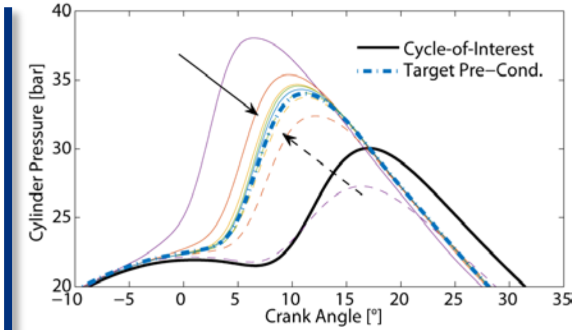
Engine Specs/Conds.

Head design	Pentroof
Displacement	0.63 liter
Bore	92 mm
Stroke	95.25 mm
CR	11.3
Speed	1200 rpm
Intake pressure	1.0 bar
T_{IVC}	~480 K
$T_{max, reformer}$	~1200 K
$\tau_{reformer}$	20 ms

Period Oxidizer Composition (%)

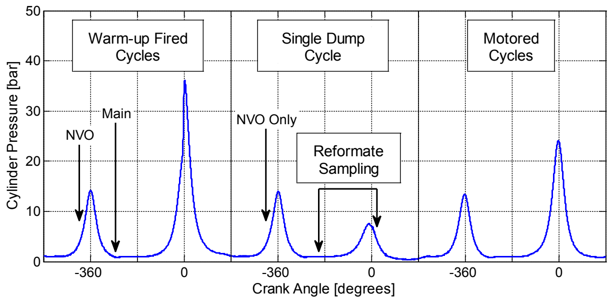
	NVO	Main
O_2	2.5	9
N_2	80	82
CO_2	8	4
H_2O	9.5	5

- In-cylinder generated reformate during NVO
  - Valve lift/timings set to retain heat & residuals
  - Pilot fuel injection
  - Low NVO O_2 w/ high temp.



- Engine performance data
  - 9-1 skip-cycle sequence
  - Generate consistent residual stream for a Cycle-of-Interest

- Reformate collection
  - Dump valve apparatus
  - Custom sampling sequence
  - Warmup cycles match Target Pre-Cond. cycles



Fuels

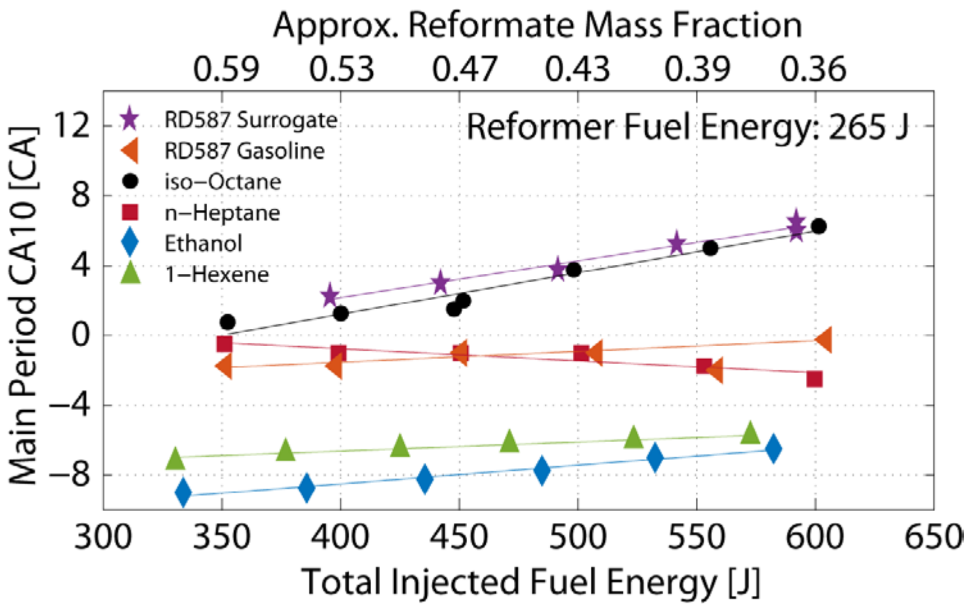
iso-octane (iso-paraffin)
n-heptane (normal paraffin)
ethanol (alcohol)
1-hexene (olefin)
cyclohexane (cycloalkane)
toluene / n-heptane (aromatic)
RD587 research gasoline
RD587 surrogate (89 AKI)
(iO: 54.9%, nH: 11.6% Tol: 18.9%, EtOH: 9.9%, 1-Hex: 4.7%, by Vol.)

- Reformate speciation
  - Neat gasoline component fuels
  - Gas chromatography (GC):
    Energy analysis
  - Photoionization mass spec (PIMS):
    Auto-ignition chemistry modeling

Accomplishment: Impact of NVO generated reformate on main-period performance observed for several fuels

Goal: Quantify impact of reformate addition on main-period combustion phasing.

- Sweep of total fueling rates with a consistent NVO reformate stream
  - NVO fueling: 265 J, Duration: 150 CA
  - remaining fuel injected in the main
  - fixed intake temp. for each fuel that phases combustion near TDC



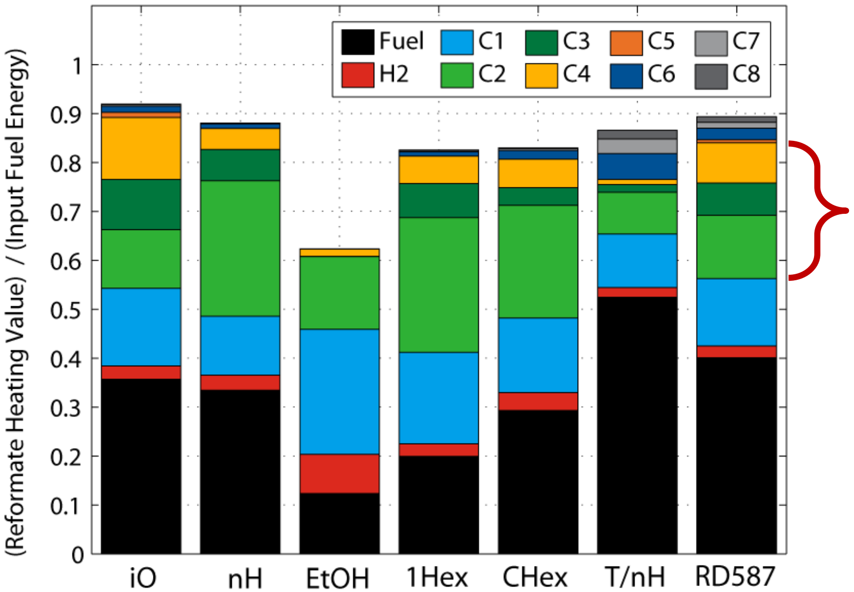
- At ***lower*** fueling rates, CA10 ***advances*** for both the gasoline and surrogate
  - everything else being equal, **lower ϕ** normally **increases auto-ignition** delays
- Similar behavior observed for engine fueled by neat surrogate components
  - exception is n-heptane,: **consistent w/ significant low-temp. heat release**
  - higher fuel stream reformate mass fraction with lower fueling rates

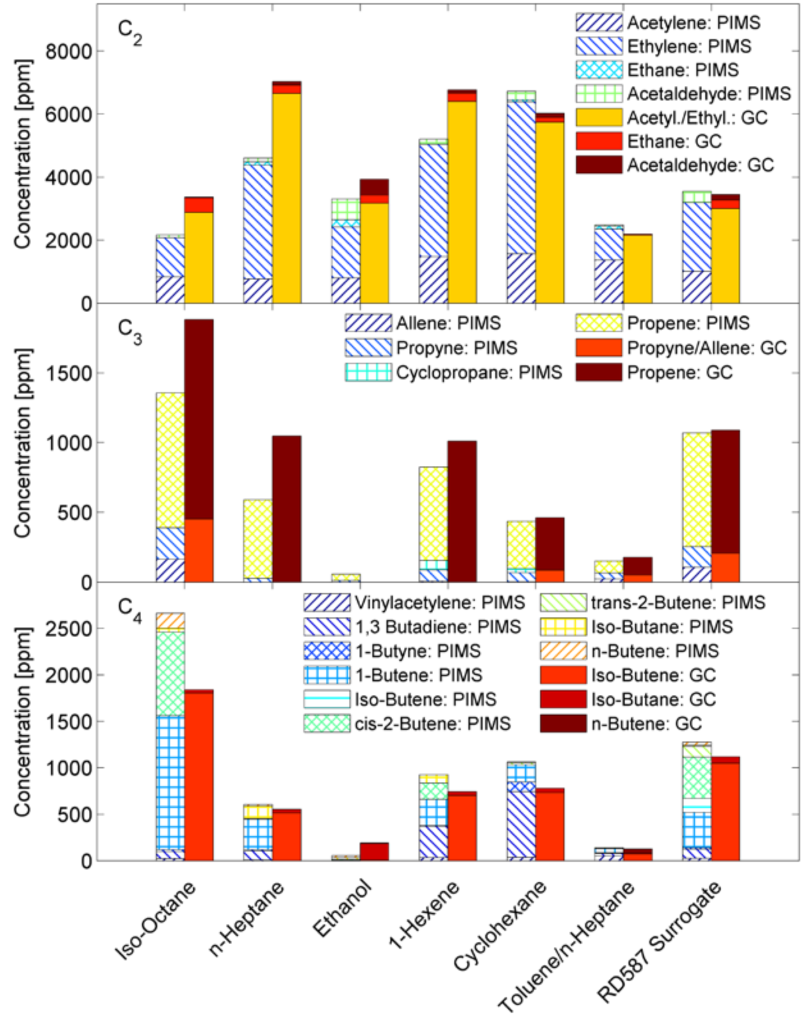
Impact: NVO generated reformate can accelerate auto-ignition chemistry for low-load LTGC where combustion stability is problematic.

Accomplishment: Characterized NVO reformate constituents for representative gasoline fuel components

Goal: Speciate reformate composition for each fuel.

- **GC**: characterize fuel energy distribution
  - ~90% fuel energy recovery (~60% for ethanol)
  - most energy from parent fuel, CO, H_2, & small HC
- **PIMS**: find species that influence auto-ignition
  - higher fidelity speciation relative to GC results

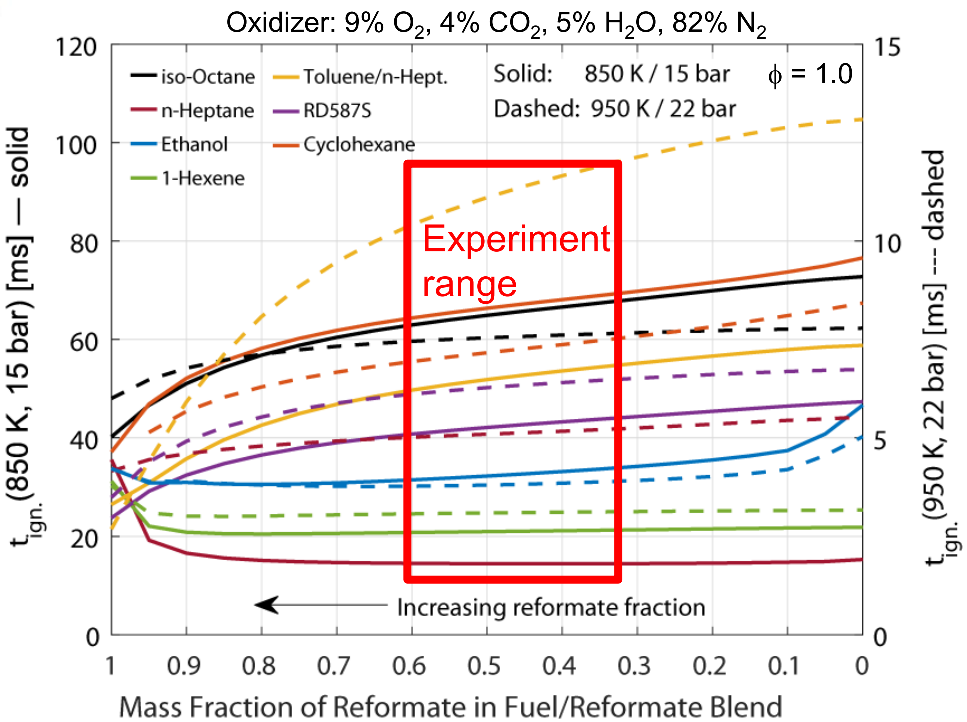




Impact:** **Results enable a systematic evaluation of each constituent's importance on auto-ignition chemistry via kinetic modeling and an ability to assess reformate composition predictions

Accomplishment: Chemistry modeling used to identify impact of reformate species on auto-ignition kinetics

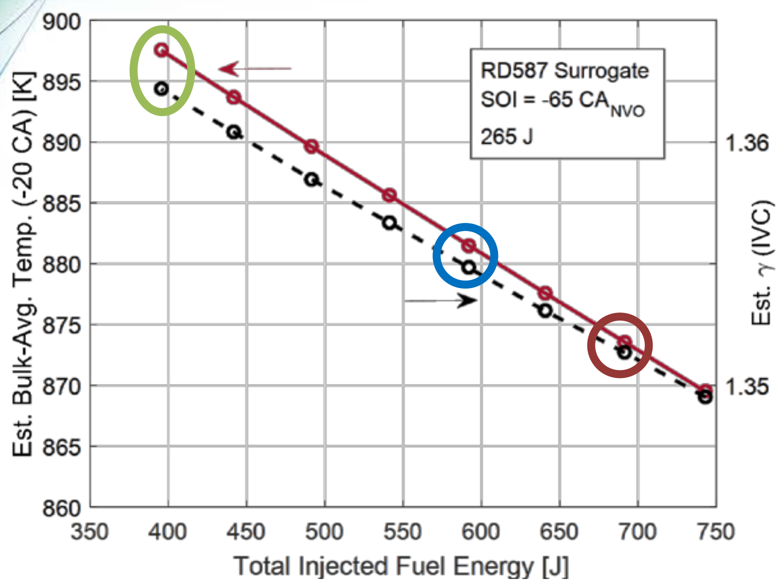
***Goal:** Leverage detailed kinetic modeling to clarify the influence of reformate addition on auto-ignition chemistry for each fuel.*



- Isochoric single-zone reactor model
  - LLNL gasoline surrogate mech.
  - PIMS measured reformate
  - GC measured oxidizer
  - Press./temp./composition cover range of in-cylinder conditions at auto-ignition
- Faster gasoline surrogate auto-ignition w/ increased reformate fraction
  - similar behavior for “high-octane” fuels
  - reactivity decreases for “low-octane” fuels
  - n-heptane sensitive to NTC chemistry
- Rapid advance of ethanol auto-ignition w/ small reformate fraction increase
  - levels off w/ higher reformate fractions

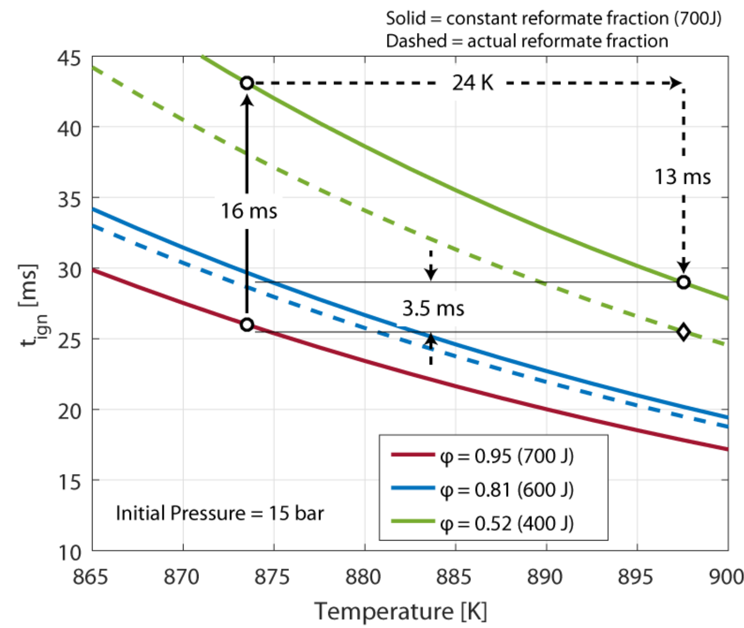
***Impact:** Select, short-chained, unsaturated HCs (<u>acetylene</u>, <u>vinyl-acetylene</u>, <u>allene</u>) and <u>acetaldehyde</u> were identified to most strongly influence increased reactivity for gasoline-like fuels.*

Accomplishment: Clarify physical and chemical effects of reformate addition on auto-ignition



***Goal:** Explain the advance of CA10 with a fixed amount of reformate addition.*

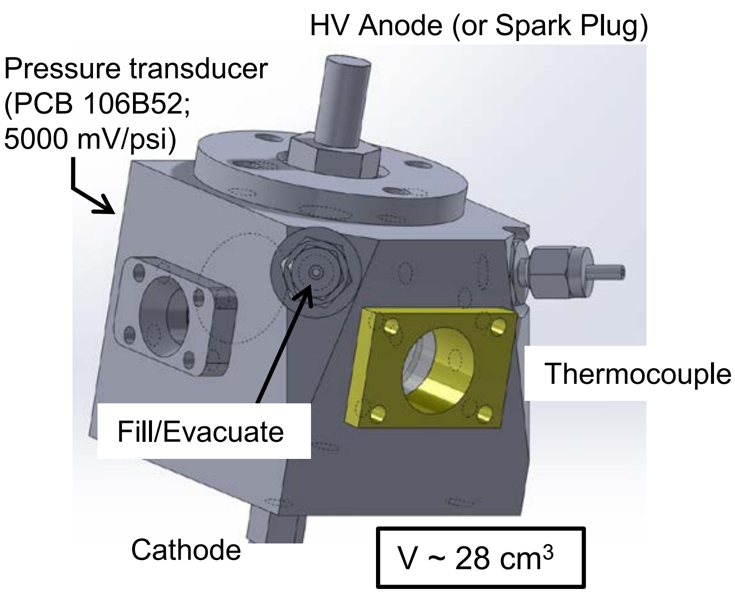
- Increased charge specific heat ratio (γ) w/ higher reformate fractions
- Less charge cooling w/ lower main-period fueling
- **Both effects increase compression bulk temp.**



- Single-zone modeling used to systematically evaluate competing effects for different fueling rates:
  - auto-ignition retards for leaner ϕ
  - most auto-ignition retard is made up if the bulk temp. accounts for **lower charge cooling and higher γ**
  - **increased reactivity** from larger reformate fractions further lead to a modest auto-ignition advance

***Impact:** Slow auto-ignition kinetics at low ϕ offset by higher bulk temp. (less charge cooling/higher γ) and increased reactivity with higher reformate fractions – explains experiment observations.*

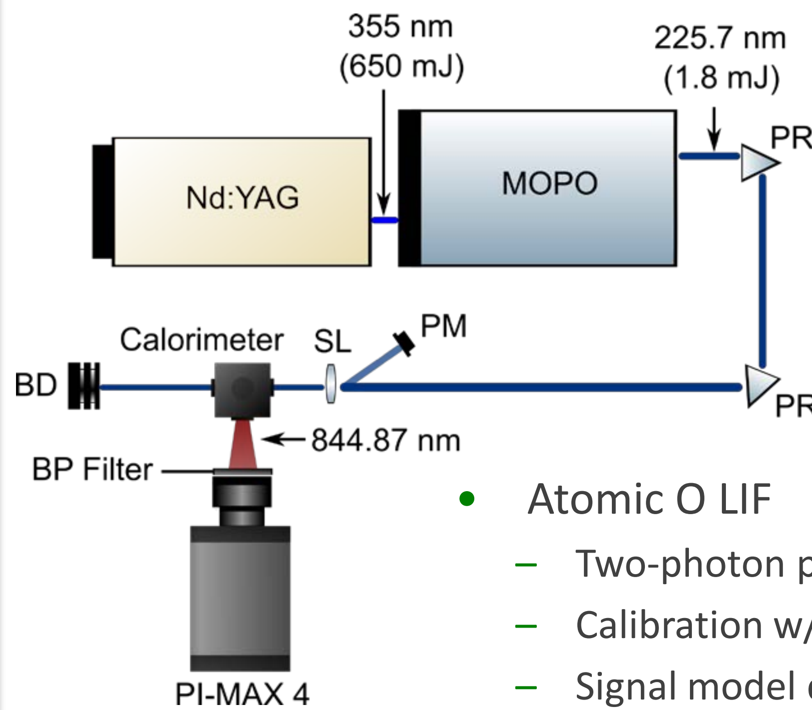
Approach: Spark calorimetry and *in situ* radical measurement for low-temperature plasma (LTP) ignition



- Custom-built calorimeter
  - High-strength quartz windows
    laser access & imaging
  - Thermal energy:
    Fast-response pressure transducer
  - Electrical pulse energy:
    In-line voltage/current probe

Transient Plasma Systems

- Pulse generator
  - ~28 kV peak voltage
  - ~12 ns FWHM pulse
  - Multi-pulse (100 μs dwell)
  - SI: NGK DR7EA, resistive
  - LTP: NGK DP7EA-9, non-resistive, (2 – 8 mm gaps)



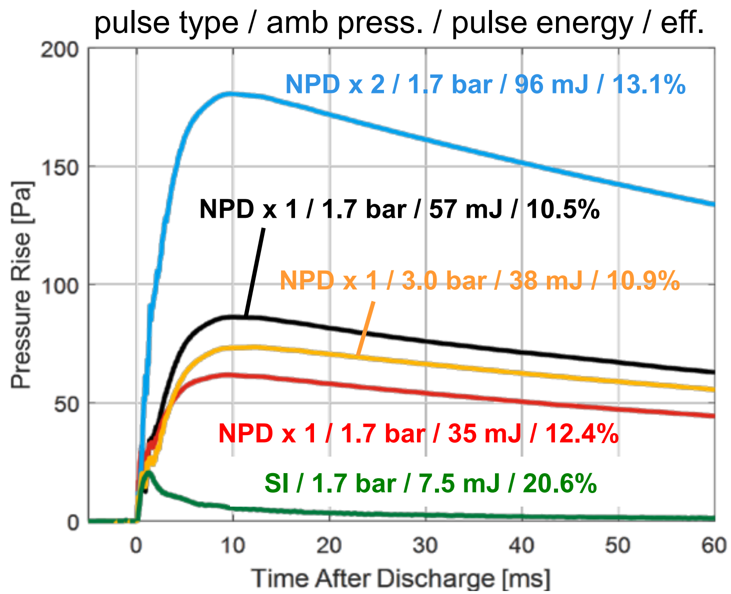
- Atomic O LIF
  - Two-photon process
  - Calibration w/ Xenon
  - Signal model developed

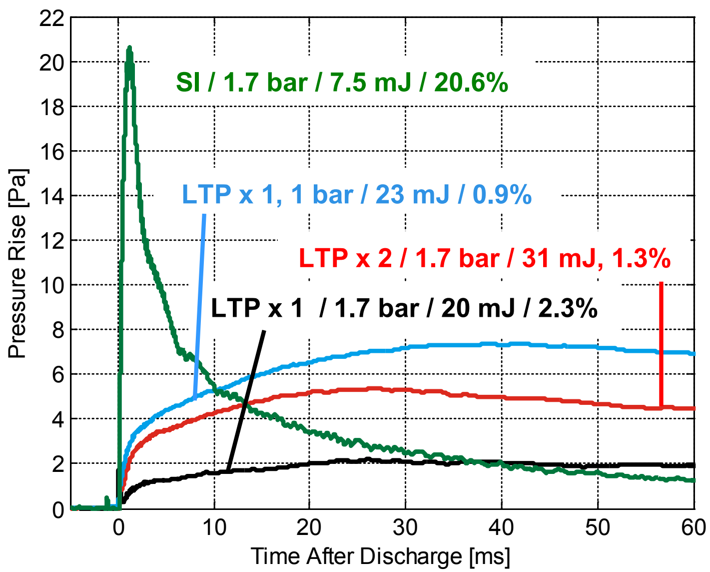
Accomplishment: Ignition calorimetry for inductive coil spark, NPD, and LTP

Goal: Quantify electrical-to-thermal energy conversion efficiency for different plasma igniters.

$$eff. \equiv \frac{E_{therm}}{E_{elec}};\ E_{elec} = \int V(t)I(t)dt\,;\ E_{therm} = \frac{Vol \cdot \Delta p}{\gamma - 1}$$

- SI: 60 J inductive coil spark - ***benchmark***
- NPD: ultra-short (~12 ns), high-voltage (~28 kV) plasma discharge ***w/ inter-electrode breakdown***
- LTP: NPD ***w/o breakdown*** (corona-like discharge)





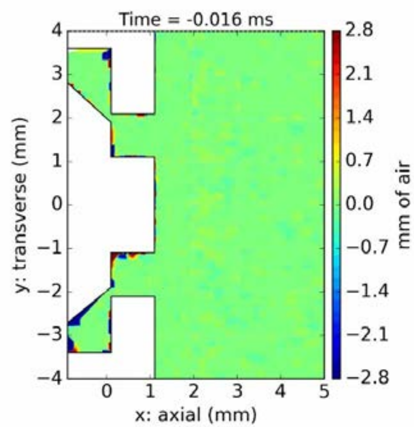
- SI: *eff.* matches literature reported values
- NPD: high secondary energy from large voltages
  - dual pulse: 2nd pulse has lower energy
- LTP: low *eff.* values relative to SI or NPD
  - continuous pressure rise long after plasma event
    - → plasma species decomposition (e.g., $O_3 \rightarrow O_2 + O$)

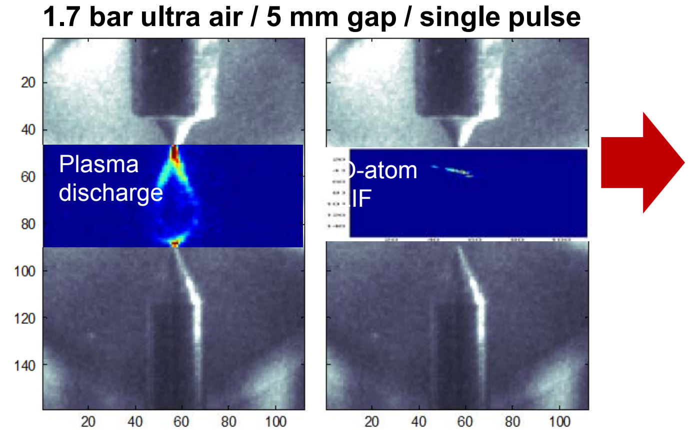
Impact: LTP energy deposition – from chemical dissociation – was low relative to SI & NPD thermal deposition.

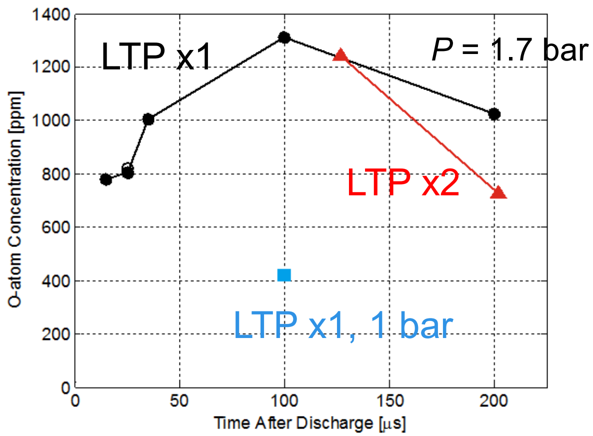
Accomplishment: O-atom laser induced fluorescence (LIF) performed during LTP ignition

Goal: Quantify the amount of LTP generated atomic O, which is an important active radical.

- Measurement just below the anode, where electric field strengths are greatest
  - ultra-air / pressures up to 4 bar / gap distances between 2 and 8 mm
  - results complement NPD x-ray radiography and modeling efforts (Argonne - AEC084)
  - 1st measurement acquired 20 µs after discharge to allow time for plasma ion recombination
- 1000+ ppm of O measured near the anode for 1.7 bar ambient (E/N = 536 Td)
  - dual pulse (100 µs dwell): O populations unchanged
  - O population more than halve at 1.0 bar despite higher E/N (887 Td)
  - atomic O nearly undetectable at 4.0 bar ambient; E/N too low (228 Td) w/ current setup







Impact: Benchmark O populations can be used to evaluate the performance of detailed CFD modeling approaches.

Accomplishment: Completed engine rebuild for advanced gasoline combustion experiments.

- Improved optical access
  - better diagnostic accessibility
  - tunable laser source for advanced spectroscopic diagnostics
- Fully automated gas handling
  - custom EGR and residual streams for skip-fired operation that match real values
- Modular design
  - rapid head/cylinder swaps
  - custom turbulent jet ignition head planned
- Higher peak pressures
  - 120+ bar
- Representative geometry
  - contoured piston
  - higher stroke/bore: 1.1

Impact: New facility enables new & better optical measurements at more relevant operating conditions.

Accomplishments: Summary

- Impact of in-cylinder generated reformate addition on LTGC auto-ignition clarified.
  - NVO generated reformate shown to accelerate auto-ignition chemistry for low-load LTGC where combustion stability is problematic.
  - Detailed in-cylinder generated reformate speciation performed for multiple fuels using a combination of GC (energy balance) and PIMS (auto-ignition chemistry) diagnostics.
  - Acetylene, vinyl-acetylene, allene, & acetaldehyde identified as the reformate constituents that most strongly accelerate gasoline auto-ignition.
  - Slow auto-ignition kinetics at low φ found to be offset by higher bulk temperatures — from lower charge cooling & higher γ — and increased reactivity w/ higher reformate fractions.
- Spark calorimetry of SI, NPD, and LTP discharges in air performed along with complementary *in situ* measurement of LTP generated atomic O.
  - Low LTP energy deposition – mostly from chemical dissociation – relative to SI & NPD.
  - Benchmark LTP discharges O measurements obtained that can be used to evaluate detailed numerical modeling of these discharges – ongoing Argonne collaboration.
  - Shared LIF and PIV data w/ Argonne for complementary SI ignition modeling.
- New engine build complete.
  - Improved capability and optical access, with more representative geometry.

Reviewer Response

R1: Previous NVO & SACI work does not always show these strategies to be the most viable for LTC.

Response: While other options can improve low-load LTC stability (e.g., PFS, RCCI, ozone addition), increasingly NVO/SACI are used to enable LTC due to their relative simplicity and robustness. Our goal is to apply unique diagnostics in custom engine platforms to learn about important physical/chemical details, with the information used to provide insight into how these systems can be optimized.

R3: Since a plasma igniter initiates a flame, how is this considered LTC?

Response: Note that several plasma ignition types exist; in FY16 we focused on SI, NPD, and LTP. LTP is of particular interest since it works by forming active species (e.g., H, O, O_3, NO) that influence auto-ignition chemistry. We seek to quantify these active species for relevant discharges.

R4: What is the impact on BTE with the use of NVO?

Response: In FY15, we found most NVO period losses resulted when the pilot fuel oxidized due high heat losses & poor expansion efficiency. In FY16, we focused on NVO periods that formed reformate w/o significant oxidation. The associated impact on ITE was characterized for a range of fuels.

R5: Work on advanced ignition has been too slow.

Response: A viable research engine platform was not available until recently. The engine build was slowed by a combination PI change at Sandia and unavoidable procurement delays with our industry partners. We nonetheless took the opportunity to craft a literature survey of recent ignition work, establish industry/research connections, and develop high-value diagnostics (e.g., O LIF, calorimetry) that will complement our engine tests going forward.

Collaborations

- National Lab
  - Oak Ridge National Lab: Joint in-cylinder reforming experiments and analysis
  - Argonne National Lab: Validation data support for advanced ignition modeling
  - Lawrence Berkeley National Lab: Detailed reformate speciation speciation at the ALS
  - Sandia BES and Plasma Sciences: Proposal to explore low-temperature plasmas physics
- University
  - USC: Ongoing collaborative research on LTP ignition
  - U. Minn.: Reformate speciation via GC / stochastic reactor modeling of NVO period
  - UC Berkeley: Modeling support for plasma ignition
  - U. Duisburg: Information sharing on reformate production (modeling & experiment)
  - Mich. State U.: Collaborative turbulent jet ignition work
- Automotive OEM
  - GM Research: Extensive interactions w/ regular teleconferences that includes: 1) technical results exchange, 2) hardware support, & 3) feedback on research directions
  - Ford Research & FCA: Discussions and guidance on advanced ignition systems
- Small business
  - Transient Plasma Systems Inc.: Electronics design and maintenance support for high-voltage nanosecond pulse generators – ongoing data sharing of plasma discharges
- DOE Working Group
  - Share research results at the DOE's Advanced Engine Combustion working group meetings.

Future Work

- Remainder of FY16
  - Perform additional spark calorimetry at more gap sizes and higher pressures
  - Extend O LIF diagnostic to planar measurements for better quantification of distributions – new optics and a more optimal laser wavelength
  - Design/fabricate new LTP and NPD spark plugs – leveraging lessons learned from the LIF/calorimetry – and evaluate the performance in the newly built engine
  - Develop a simplified stochastic reactor model (w/ U. Minn.) – that accounts for mixing and detailed kinetics – to predict NVO period generated reformate streams
- FY17 Future work
  - Acquire *in situ* measurements of LTP generated species (OH, NO, O_3) in the optical calorimeter w/ simple fuels added (<C_3) and the air diluted by representative EGR
  - Explore the use of dielectric materials to suppress NPD current flows
  - Continue systematic evaluation of different LTP and NPD plugs – particular focus on dilution tolerance extension for early DI
  - Apply optical measurements in the engine for select operating conditions with LTP and NPD ignition – high-speed and spectroscopic imaging near ignition
  - Modify spare engine head to accept a turbulent jet igniter – time permitting, perform exploratory measurements

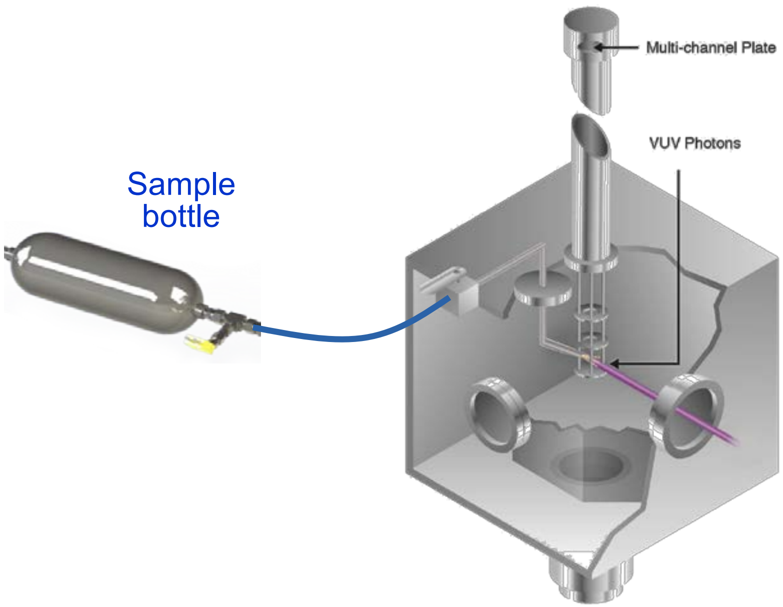
Technical Backup Slides

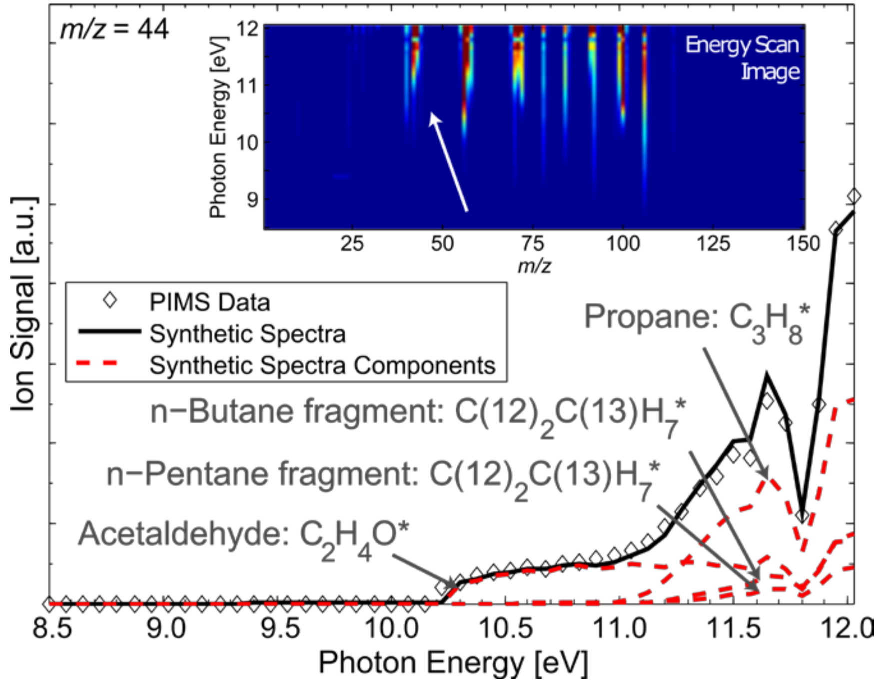
Technical Backup: Photoionization Mass Spectroscopy

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

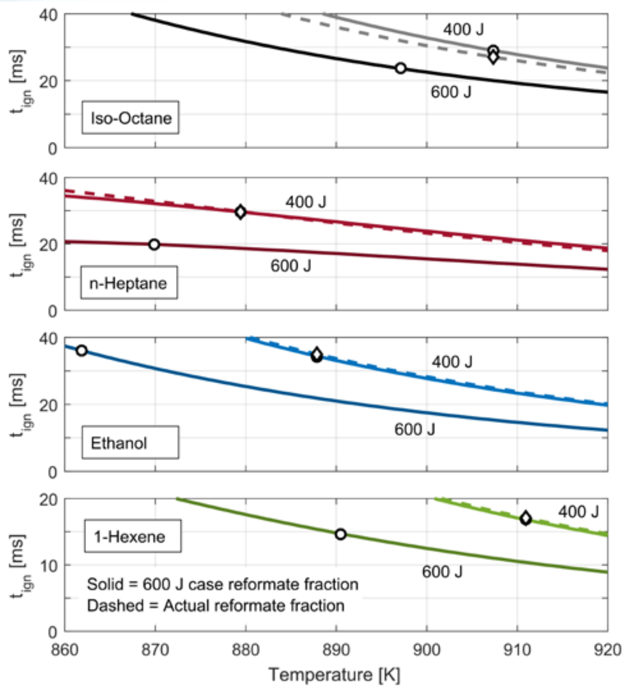
Iteratively adjusted to best fit data

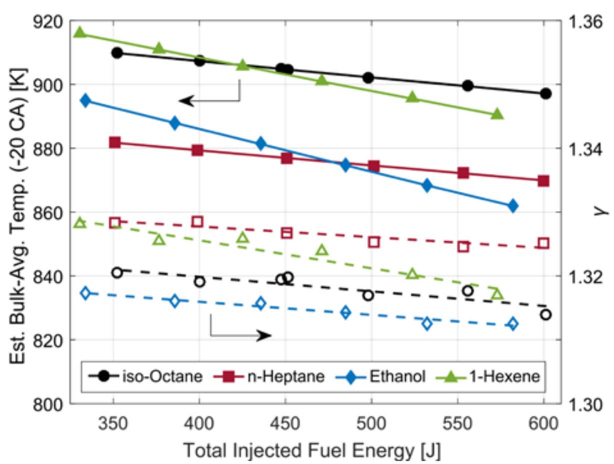
$$\sum S_{i,j,k} = \chi_k \cdot \sigma_{i,j,k} \cdot D_{i,k} \cdot \Phi_j \cdot PD_j^{-1} \cdot SW_j \cdot C_j$$

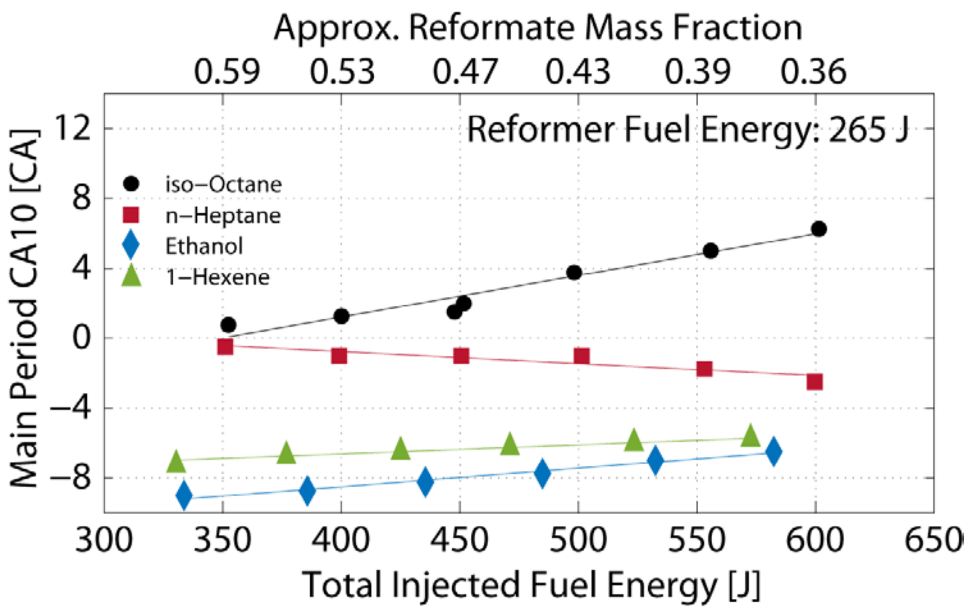




Technical backup: Performance for gasoline fuel components





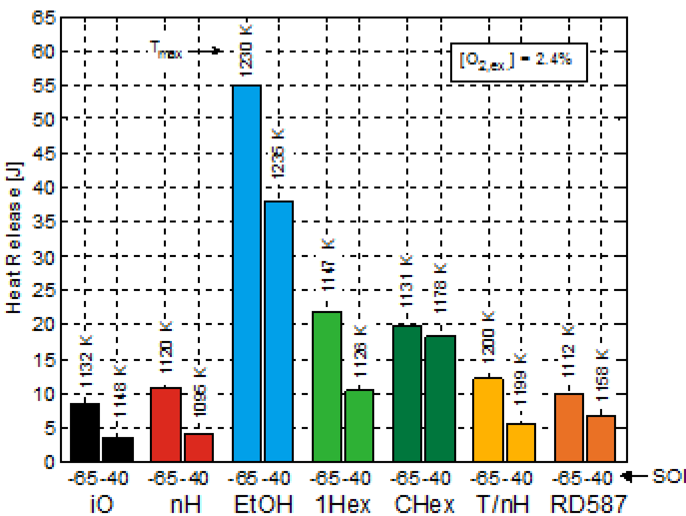


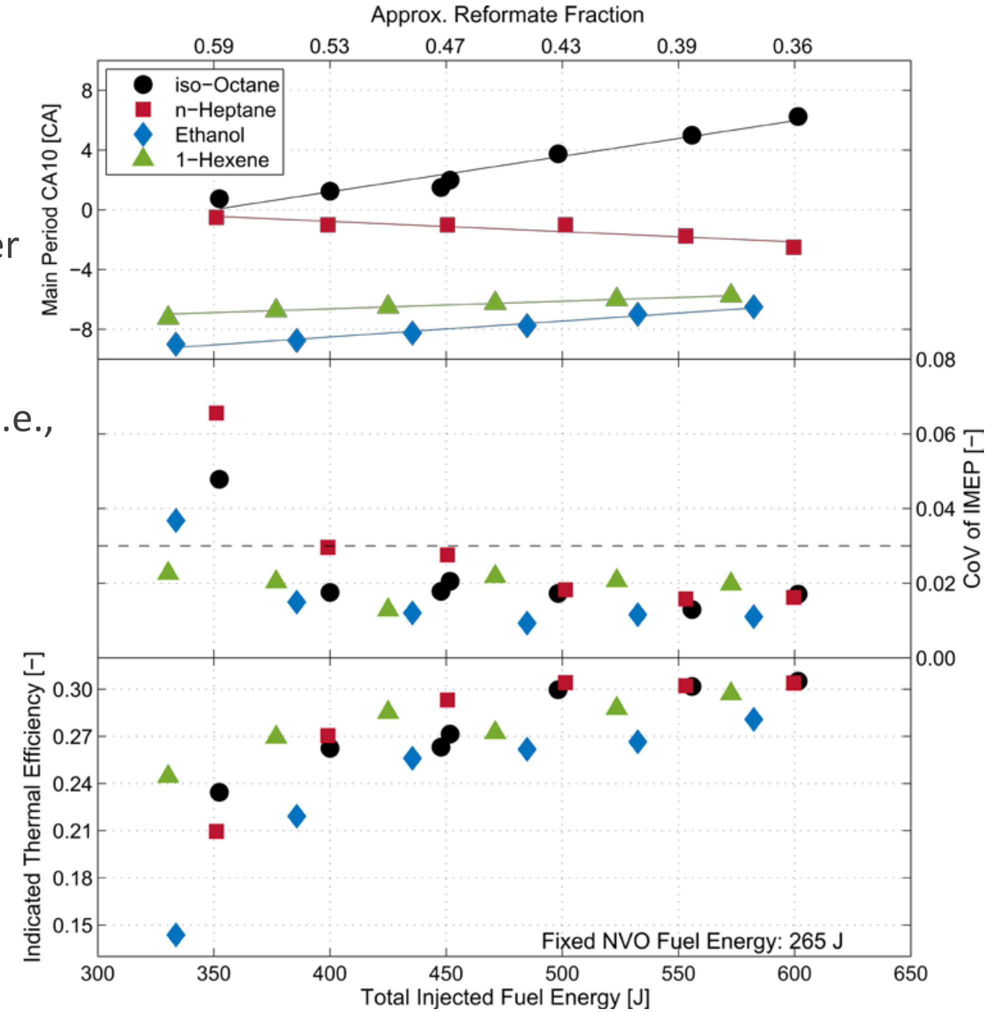
Modeled reformate effect on auto-ignition relative to RD587 gasoline surrogate

	Charge Cooling	γ	Reactivity
Iso-Octane	Neutral	Small	Neutral
n-Heptane	Neutral	Small	Small
Ethanol	Large	Neutral	Small
1-Hexene	Neutral	Large	Small

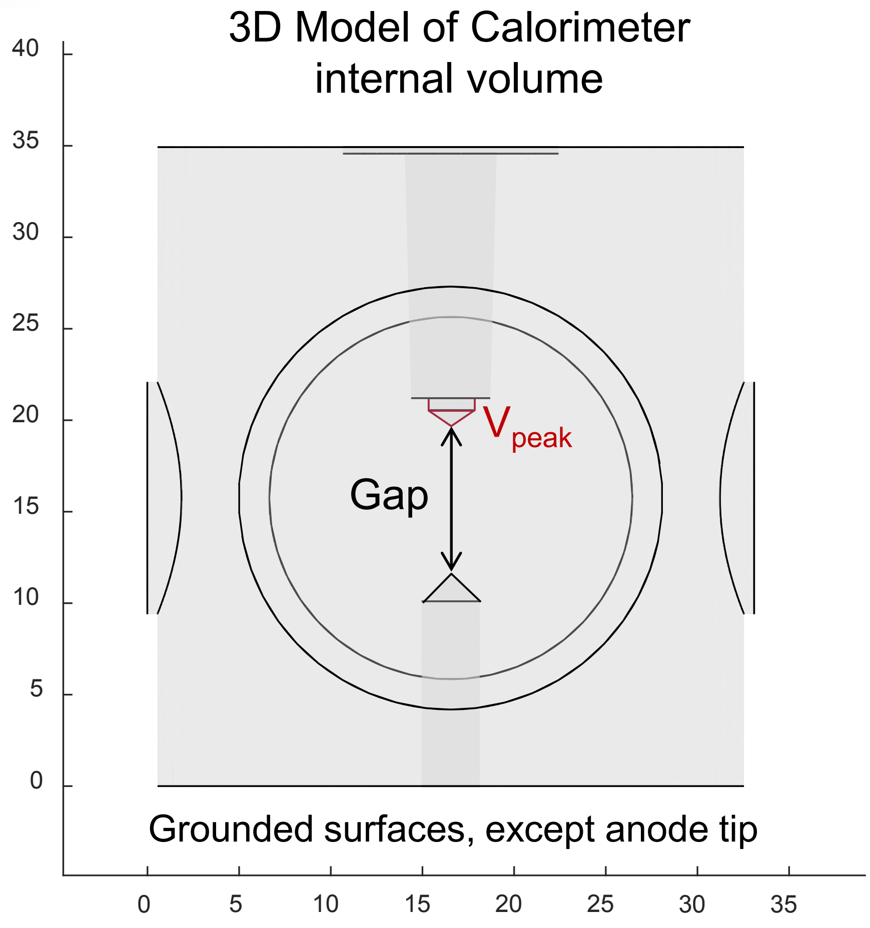
Technical backup: Performance for gasoline fuel components

- CoV below 3% for most conditions
  - exception for 350 J fueling
- ITE highest for n-heptane & iso-octane
  - slight ITE reduction for 1-hexane at higher fueling rates
  - larger ITE reduction for ethanol
  - fuels had the highest NVO heat release (i.e., less fuel energy available for the main)





Technical backup: MATLAB PDE Toolbox used to simulate E-field: peak E-field likely did not change with gap



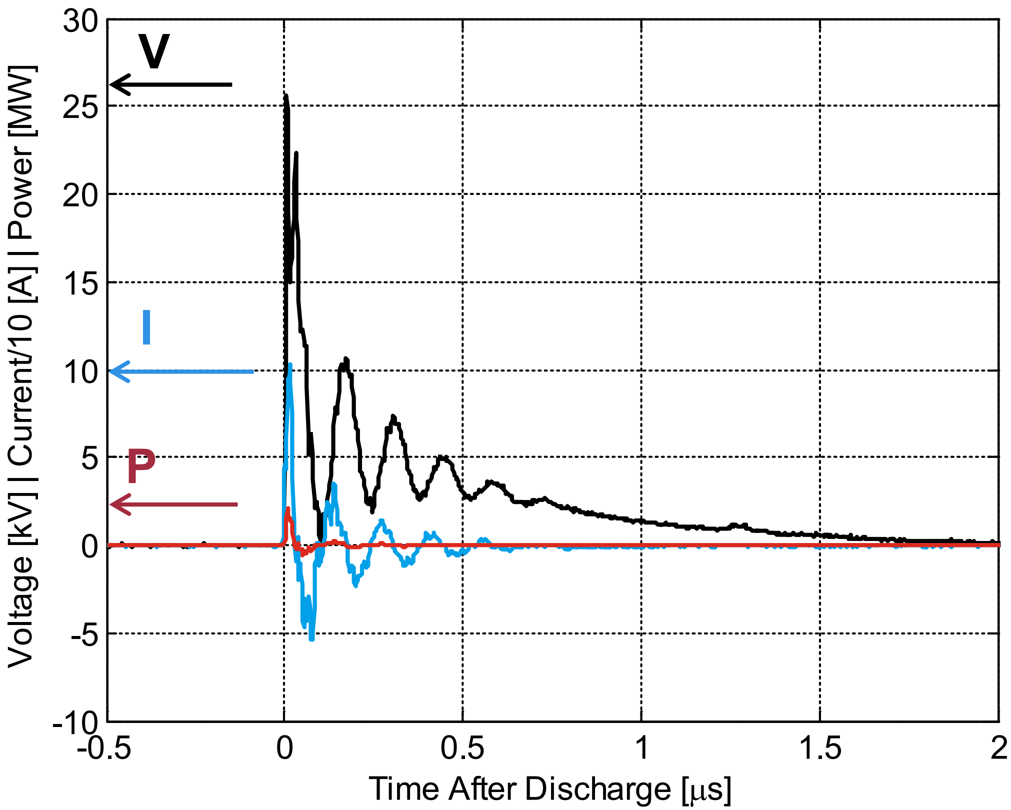
Simulations performed using permittivity of air, V_{peak} from experiments (~25 kV)

Gap [mm]	E_{anode} [10^7 V/m]	*P* [bar]	Est. *E*/*N* [Td]
8	2.17	1.0	887
5	2.23	1.7	536
2	2.23	4.0	228

Anode(x,y) = (16.55, 19.50)

Technical backup: Measurement of inline voltage, current, and resultant power during NPD/LTP calorimetry

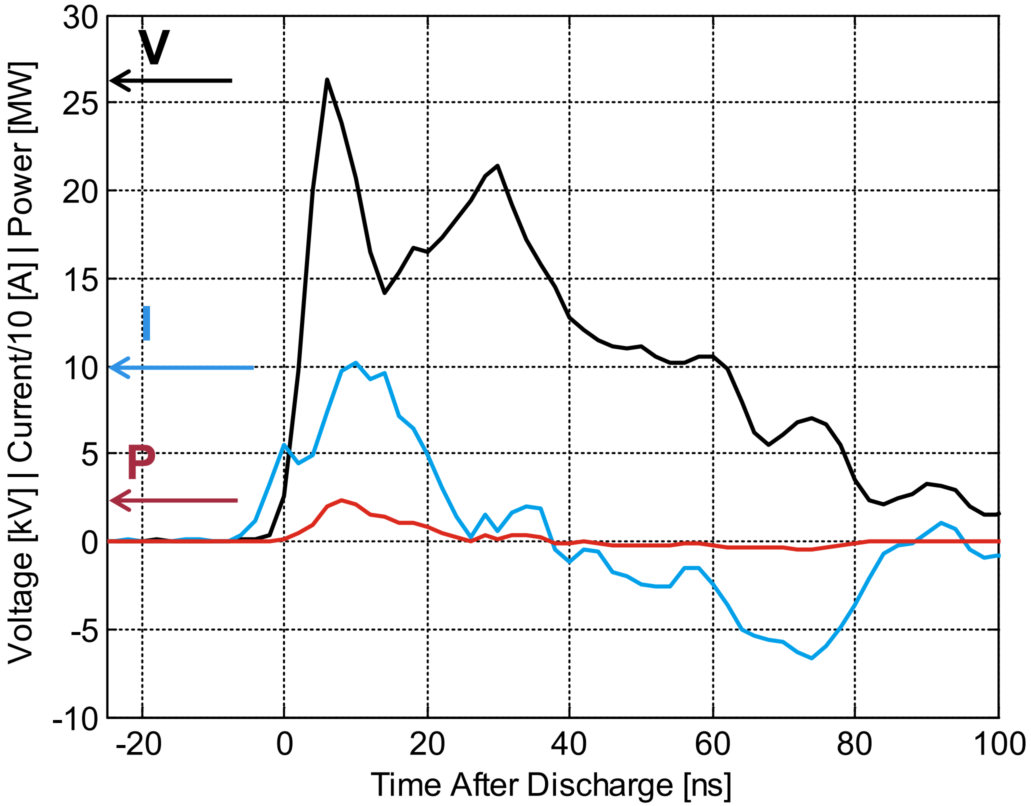
1st Pulse (19.7 mJ)



P = 1.7 bar

Technical backup: Measurement of inline voltage, current, and resultant power during NPD/LTP calorimetry

1st Pulse (19.7 mJ)



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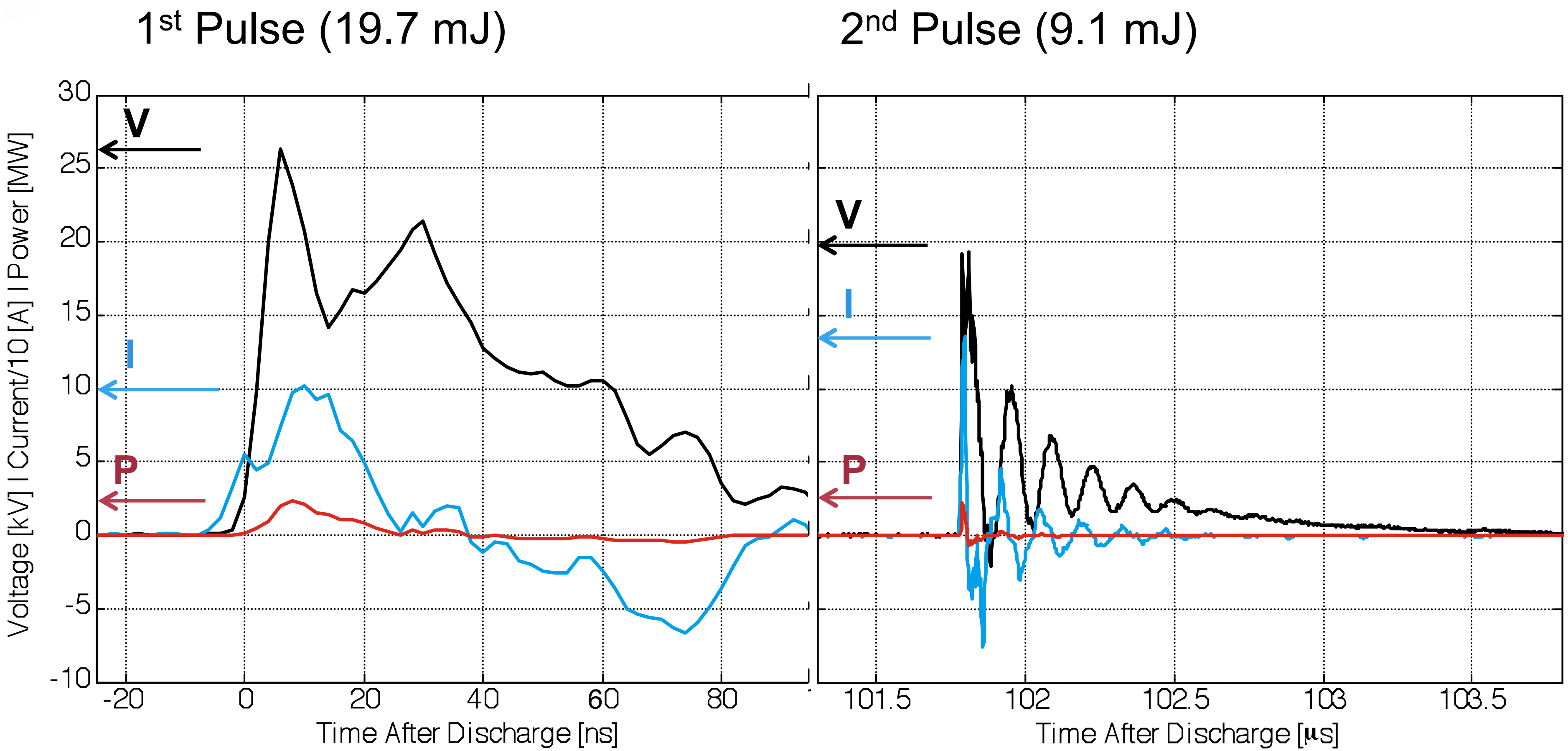
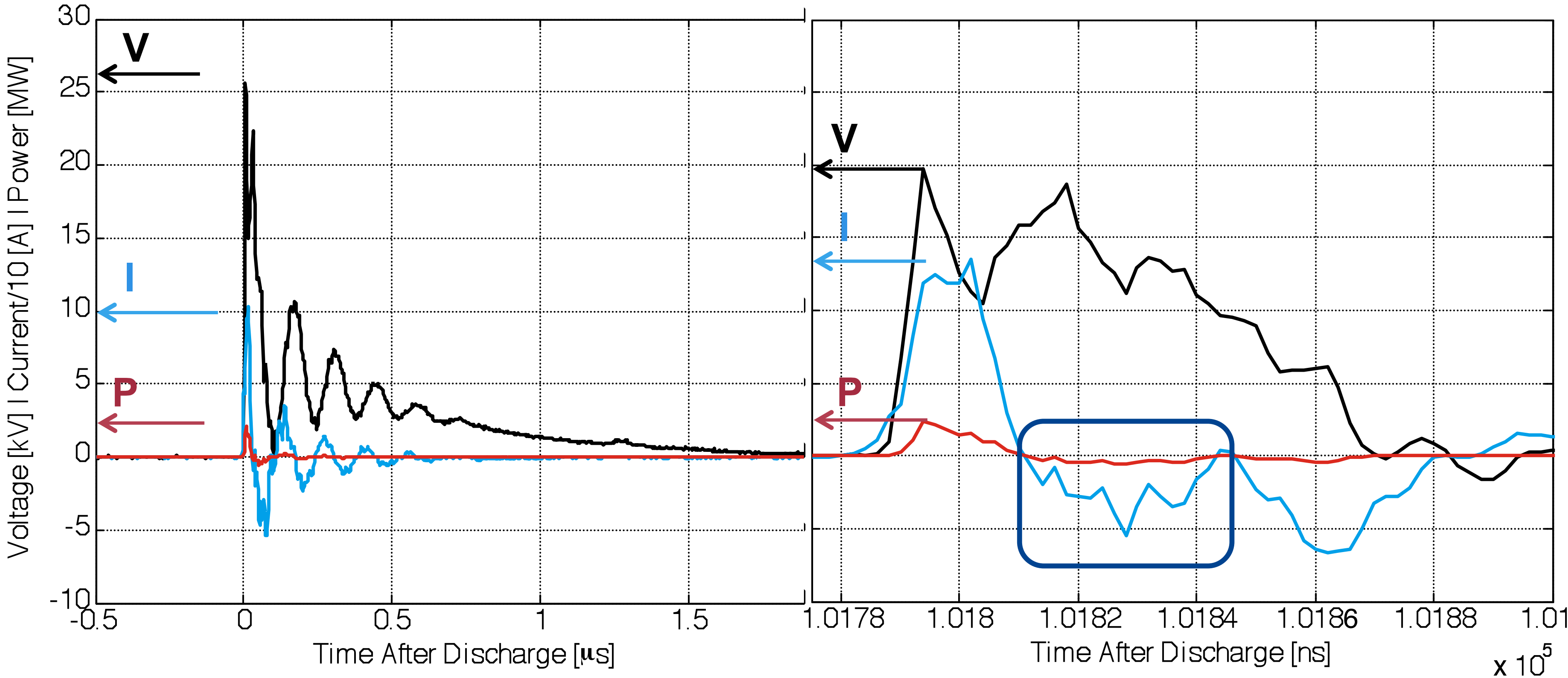


P = 1.7 bar

Technical backup: Measurement of inline voltage, current, and resultant power during NPD/LTP calorimetry

1st Pulse (19.7 mJ)

2nd Pulse (9.1 mJ)



P = 1.7 bar