COMBUSTION RESEARCH FACILITY

Automotive HCCI Engine Research

Richard Steeper
Sandia National Laboratories

2013 DOE Vehicle Technologies Annual Merit Review
Arlington, VA
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Program Manager: Gurpreet Singh
DOE Office of Vehicle Technologies

Project ID: ACE006

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
- FY12 funding: $680k
- FY13 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.
- Target goals for Advanced Combustion R&D (2015):
  - 25% Gasoline fuel economy improvement;
  - Achieve Tier II, Bin 2 emissions with < 1% thermal eff. penalty.

Partners

- Project lead: Richard Steeper, Sandia
- Industry:
  - GM & Ford: technical guidance
  - 15 Industry partners in DOE Working Group.
- University/National Lab:
  - Oak Ridge National Lab
    - Joint experiments on NVO fueling
  - Lawrence Livermore National Lab:
    - Chemical analysis, chemical kinetics models
  - 6 National labs and 5 universities in DOE Working Group.

Relevance: Objectives and Milestones

» Overall objective:

- Expand our fundamental understanding of low-temperature combustion (LTC) processes needed to achieve clean and fuel-efficient automotive HCCI engines.

» Specific objectives:

- Characterize negative valve overlap (NVO) strategy for control of HCCI combustion under low-load conditions.
  - Milestone: Perform engine experiments to identify chemical effects of NVO fueling on main combustion phasing.
  - Milestone: Perform seeding experiments to quantify combustion enhancement due to specific NVO product species.
- Apply computer models to understand and guide our automotive HCCI experiments.
  - Milestone: Apply Chemkin-Pro piston/cylinder model of main combustion to clarify NVO enhancement chemistry.

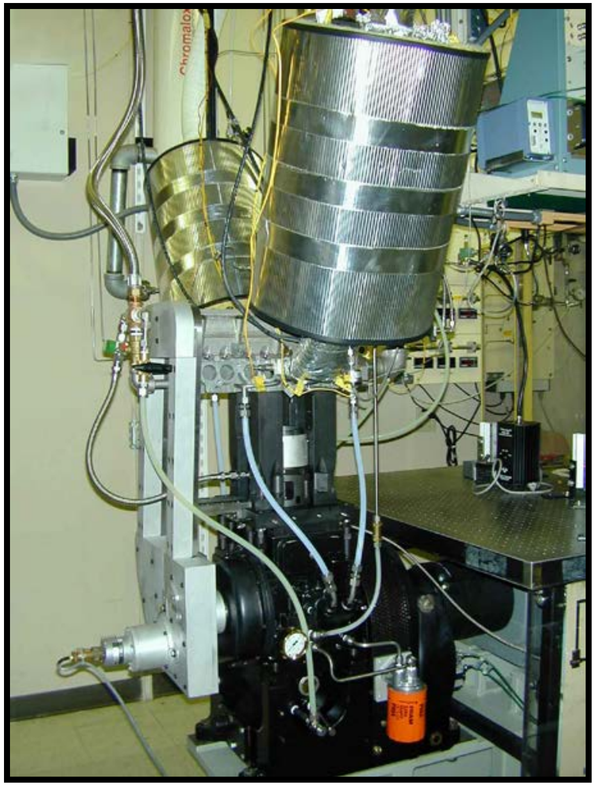
Approach

» Perform <u>experiments</u> in an optical engine equipped and configured for automotive HCCI combustion strategies.

» Develop and apply <u>diagnostics</u> to acquire in-cylinder measurements of fundamental physical processes.

» Apply suite of <u>computer models</u> to guide and interpret engine experiments.

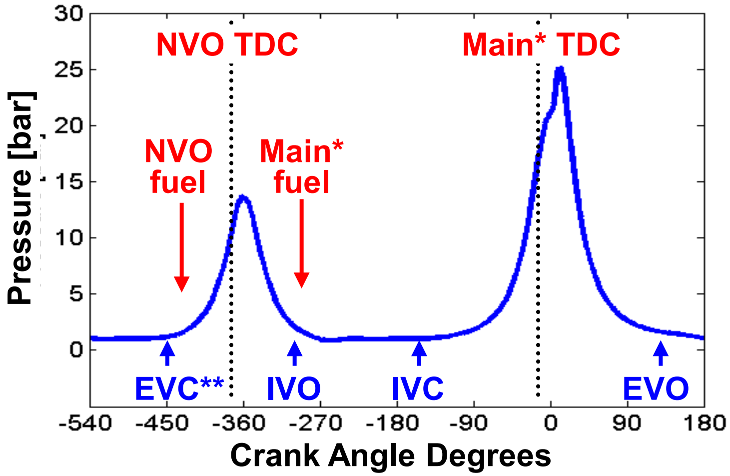
» Leverage <u>knowledge gained</u> through technical exchange with DOE Vehicle Technologies program participants.



Technical accomplishments

»Background – Gasoline HCCI-NVO research:

- NVO strategy is of current interest for SI mixed-mode engines:
  - The engines produce high specific output while in SI stoichiometric mode;
  - At low load, NVO enables HCCI combustion, thereby gaining efficiency and emissions advantages.
- Overall advantages have been demonstrated, but chemical and physical details are poorly understood.
- Determining those details will allow efficiency gains to be optimized over the widest range of conditions possible.



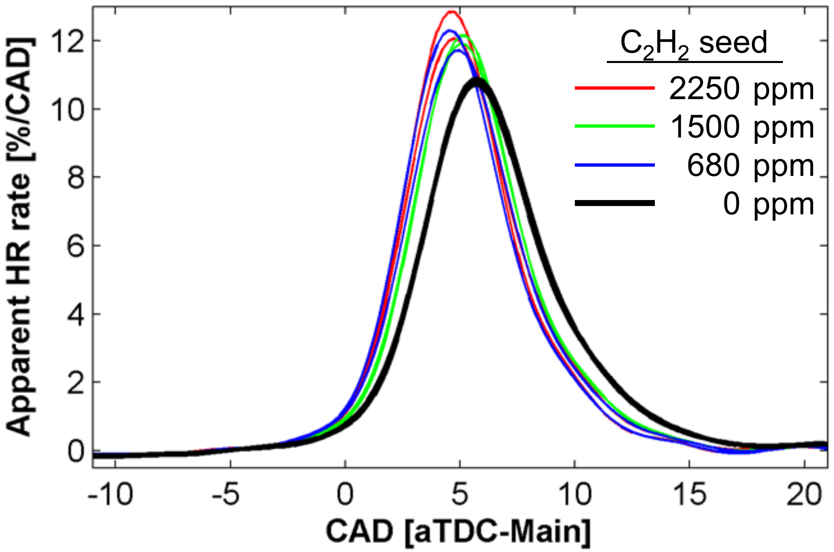
»FY13 accomplishments are divided into four topics:

- Completion of acetylene seeding study.
- Design and development of a gas sampling system for research engine.
- Deployment of sampling system to probe chemistry of NVO-fueled operation.
- Application of models to expand understanding of NVO reactions.

* *Main* is used throughout to distinguish the *Main* versus *NVO* portions of cycle.
** EVC, IVO, etc.: Exhaust/Intake Valve Closing/Opening.

Technical accomplishments: Completion of acetylene seeding project.

- Project presented in detail at last merit review.
- Final analysis completed Fall 2012.
- Results published/presented at SAE Malmo meeting.
- Observed combustion enhancement due to acetylene is relevant to our newer projects and will be referenced in this presentation.



Technical accomplishments: Implemented cylinder gas sampling system for HCCI-NVO engine.

» Previously, we have applied multiple techniques to probe engine combustion:
  - Laser-induced fluorescence, laser-absorption, high-speed imaging, seeding experiments.
  - Cylinder sampling is a natural complement:
    - Done rarely and typically limited to micro-sampling.
    - If done well, can provide desired details of NVO chemistry.

» We designed a cylinder-dump system that captures cylinder contents during main compression. This is convenient since:
  - Any NVO reactions are quenched during intake, so fast sampling is unnecessary.
  - NVO species are diluted, but details of this mix (IVC composition) are desired for analyzing chemical effects of NVO on main combustion.

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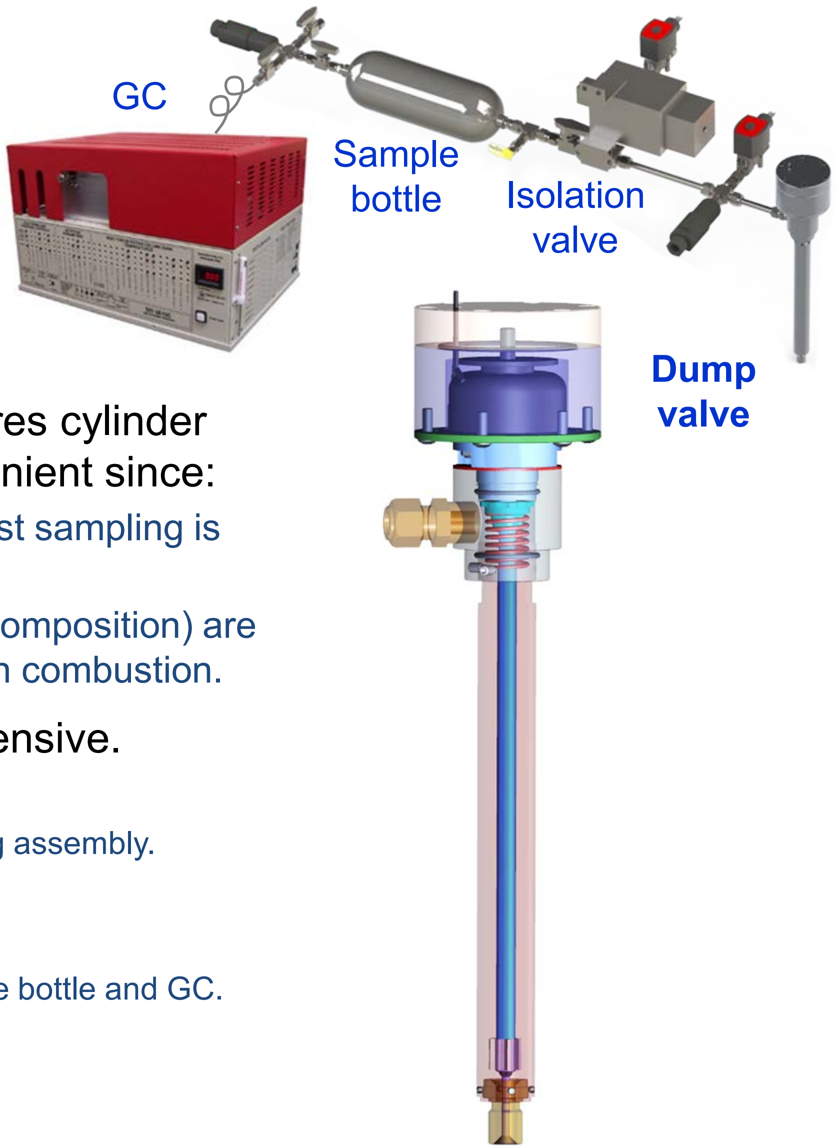

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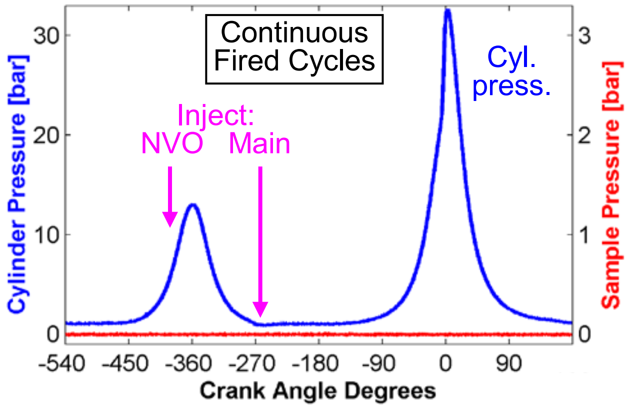
» Completed system is relatively simple and inexpensive.
  - Dump valve:
    - Custom valve, but stock spark-plug threads and stock spring assembly.
    - Driven by low-voltage, commercial solenoid;
  - Gas manifold:
    - Heated tubing and hardware connects dump valve to sample bottle and GC.
  - Gas chromatograph (GC):
    - Twin detectors (FID/TCD*) and columns.

* FID/TCD: Flame Ionization and Thermal Conductivity detectors

Verified performance of dump valve during fired NVO operation.



» Above pressure record illustrates the sequence of cycles used for sampling:
- Once steady firing is established, we perform the single-cycle sample by cutting main fuel inject and opening dump valve.
- Pressure in engine cylinder drops during dump cycle and pressure in collection manifold spikes.

» System collects significant fraction of cylinder gas contents at IVC:
- 150-300 ml per dump event (i.e., quarter to half the contents).
- Sample bottle accumulates multiple dumps, assuring a cycle-averaged composition.

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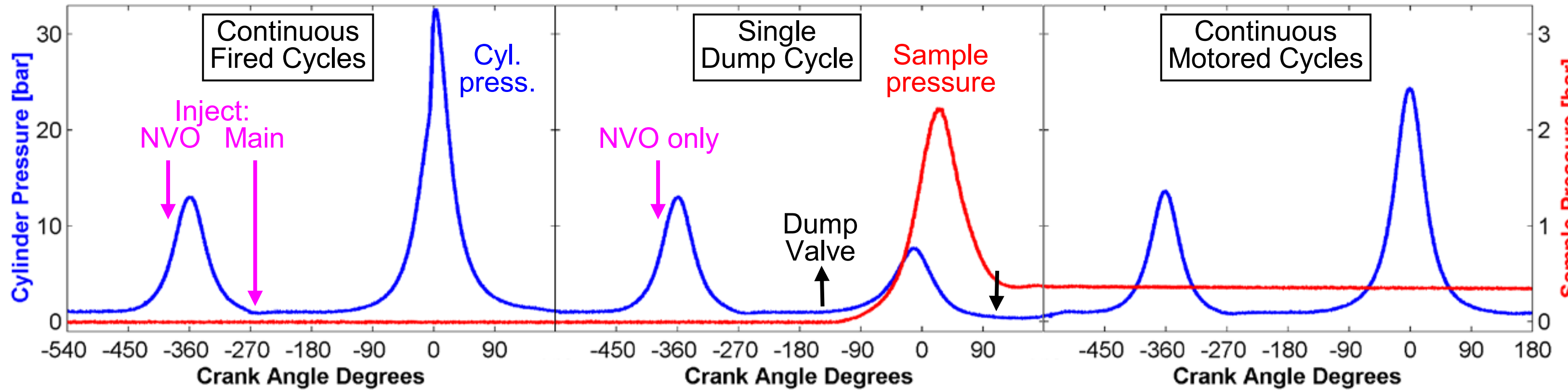

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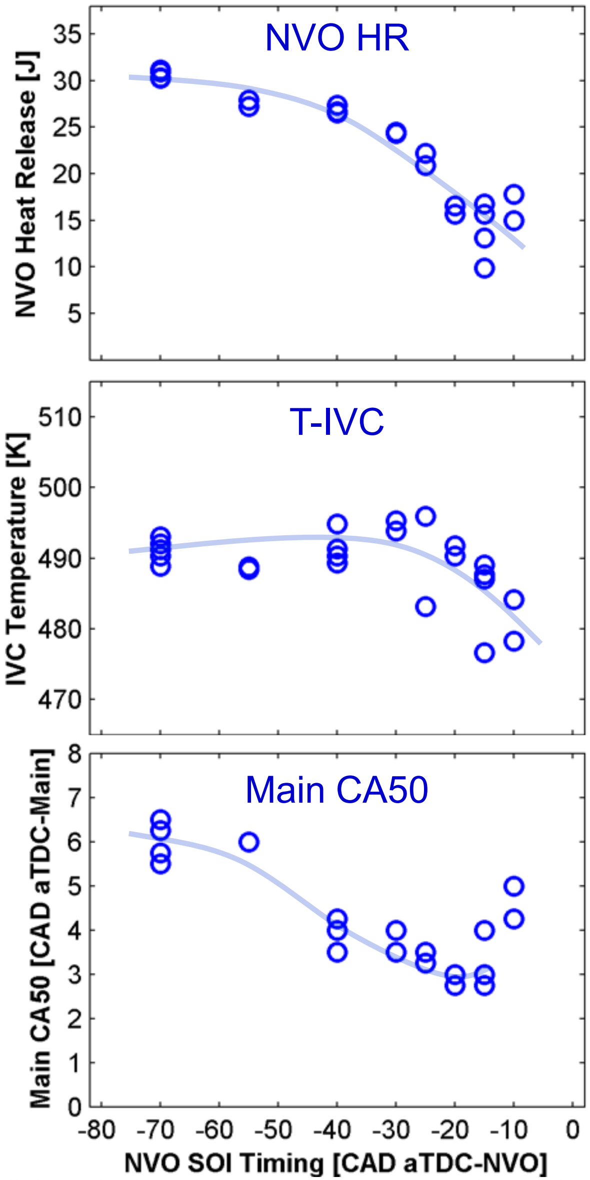
Technical accomplishments:
Series of NVO sampling experiments completed.

- Experiments designed to measure effects of NVO fueling as injection timing is varied (SOI sweep):
  - Results show strong trends in both engine performance and sample composition.
- Plots summarize engine performance as SOI is retarded:
  - Heat release during NVO drops steadily as available reaction time decreases and piston wetting increases;
  - Temperature at IVC falls off as SOI approaches TDC;
  - Despite both of these effects, which should act to *retard* main combustion, location of 50% burn (CA50) primarily *advances*.
- Results reinforce conclusions from past experiments:
  - Observed advance of CA50 with SOI retard suggests a chemical rather than thermal effect of late NVO fueling.
  - Cylinder sampling is meant to clarify that trend…

<u>Low-load operating conditions:</u>

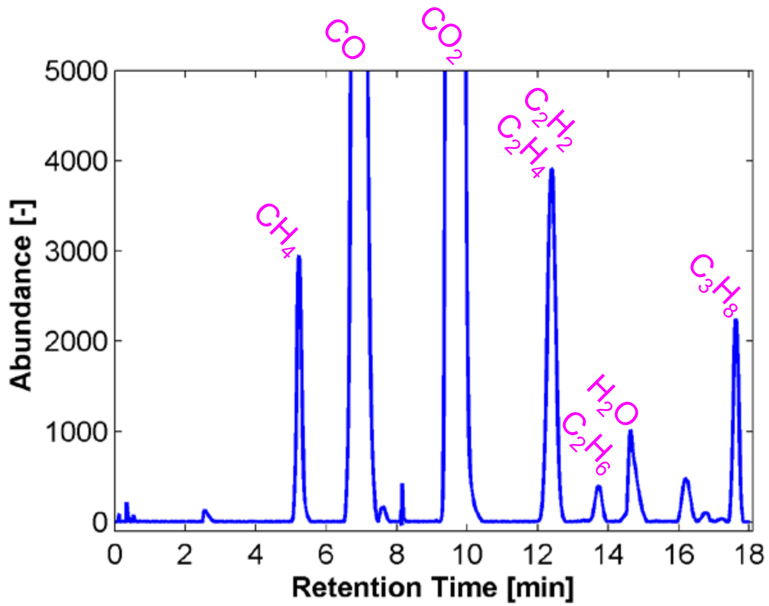
- All-metal engine
- NVO: 150 CAD; RGF ~ 50%
- T_{INTAKE} = 120 °C
- Split inject: 1.2 + 8.4 mg iso-octane; ϕ = 0.6
- IMEP = 190 kPa; COV < 3%



Speciation of NVO products performed using multiple GCs.

» We calibrated our GC/FID to speciate fixed gases and small hydrocarbons.
- Repeated chromatograms were run following each experiment.
- Measurement repeatability is better than ±10% for all but weakest peaks.
- Trends are summarized on next slide.

» Additionally, samples were analyzed at LLNL in collaboration with Lee Davisson:
- GC/mass spectrometry used to extend the list of identified species, including:
  - 2,2,4-Trimethylpentane (parent fuel),
  - Formaldehyde and acetaldehyde,
  - Propene and 2-methylpropene.



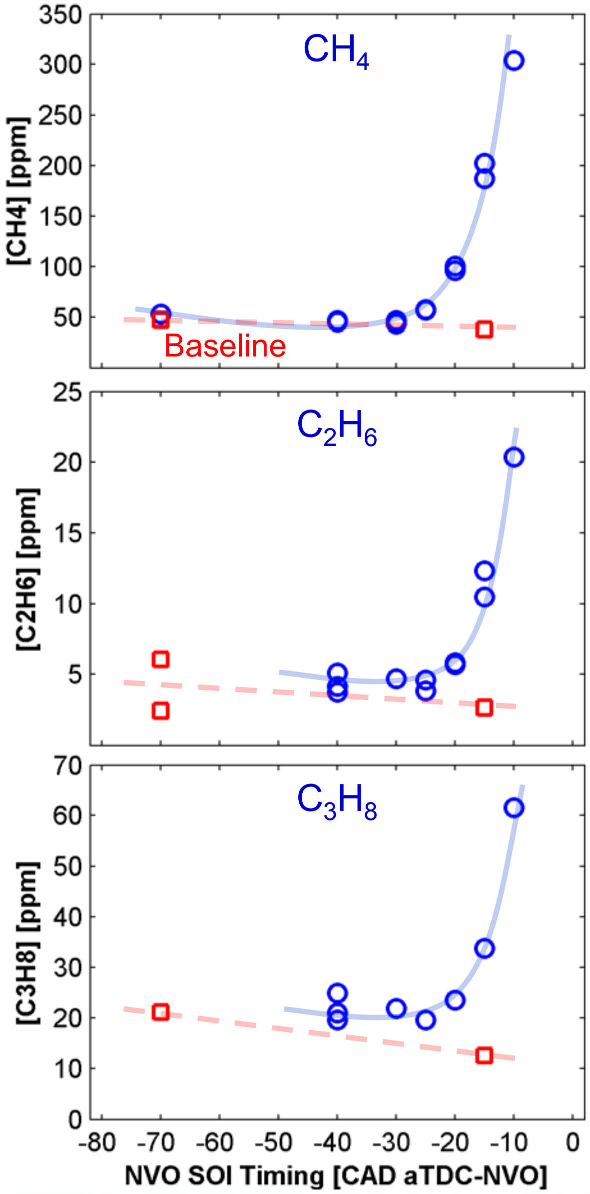
NVO product composition correlates strongly with SOI.

» Baseline composition for comparing with NVO products obtained by modifying the dump cycle:
  - By suppressing both NVO and main fuel injections (instead of just main), baseline represents species carried over from the previous main combustion.

» For early-to-mid SOI timing, NVO production of small alkanes is minimal, adding little to the baseline.

» However, for NVO injections later than 30 degrees bTDC, there is a distinct spike in production.

» This rise in composition adds to our list of observed trends associated with late NVO injection:
  - Trends in engine performance data,
  - Trends in laser-based measurements of CO,
  - Observations of piston wetting and pool fires.



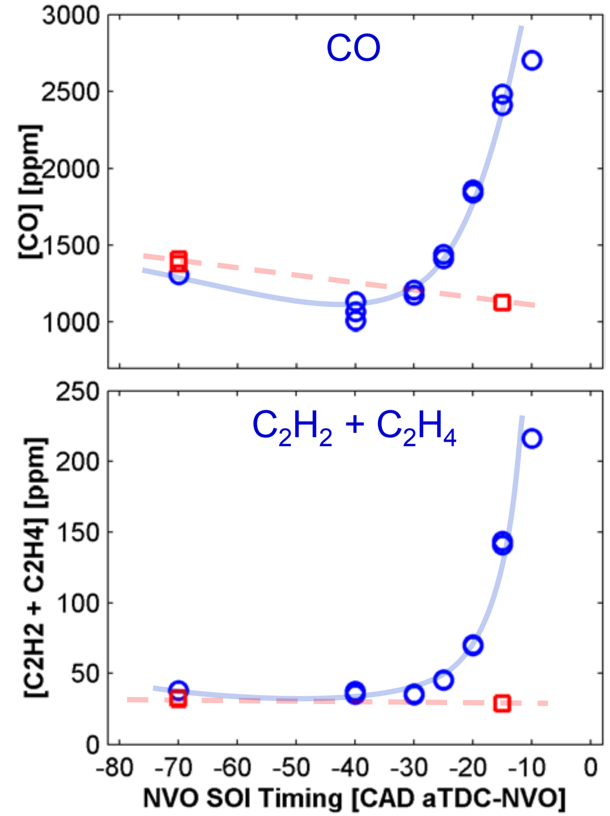
Other NVO product species of interest.

» Carbon monoxide:
- CO (and C_2H_2) profiles mirror trends of alkanes.
- Prior seeding experiments determined that increased [CO] at IVC has little influence on main combustion phasing. But CO data are needed as a metric of reaction extent during NVO.
- Further, GC data show excellent agreement with prior in-cylinder measurements of CO made using a laser-absorption diagnostic.*

» Acetylene:
- Past experiments determined that 680 ppm C_2H_2 seeded into the intake enhances main ignition.**
- While our sampling experiments do not show [C_2H_2] as high as that, we still see a correlation of increasing C_2H_2 production and advancing CA50 with late NVO fueling.

» Formaldehyde:
- Data limited, but [CH_2O] decreases for late NVO fueling.

» Significance of sampling experiments:
- Our SOI sweep data contribute to evidence of chemical effects of late NVO fueling on main combustion phasing;
- Data can assist the tuning of NVO reaction models;
- Details of composition at IVC facilitate modeling main combustion…



* SAE Int. J. Engines, doi:10.4271/2010-01-2254; ** SAE Int. J. Engines, doi:10.4271/2012-01-1574

Technical accomplishments: Model development and application.

»We employ multiple engine models to guide and interpret experiments:

- In-house cycle-temperature analysis program.
- Chemkin Pro piston/cylinder reactor model.
- GT Power engine system simulation.
- KIVA CFD/kinetics model of optical engine created by LLNL and University Of Wisconsin.

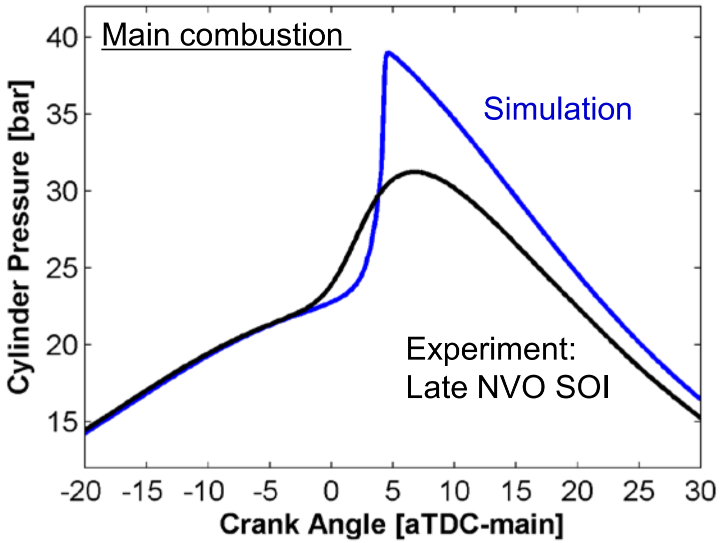
»Accomplishments this year include:

- Adapting our cycle-temperature program to estimate engine parameters for cylinder sampling experiments and modeling.
- Applying Chemkin model to simulate enhancement of main combustion by NVO products…

Chemkin simulations make use of cylinder sampling data.

» Chemkin simulation setup:
- Single-zone piston/cylinder model of IVC to EVO.
- LLNL detailed iso-octane mechanism.
- Initial composition (IVC) based on sampling results.

» Single-zone model is simplistic, but results prove useful:
- Late-injection experiment shown along with simulation.
- Temperature offset (55 K) is needed to match CA50s.
- Initial composition of simulation = major species plus the measured trace species shown in table.



Sampling experiment trace species:

• C_2H_2	142 ppm
• CH_2O	122 ppm
• CH_4	195 ppm
• C_2H_6	10 ppm
• C_3H_8	34 ppm

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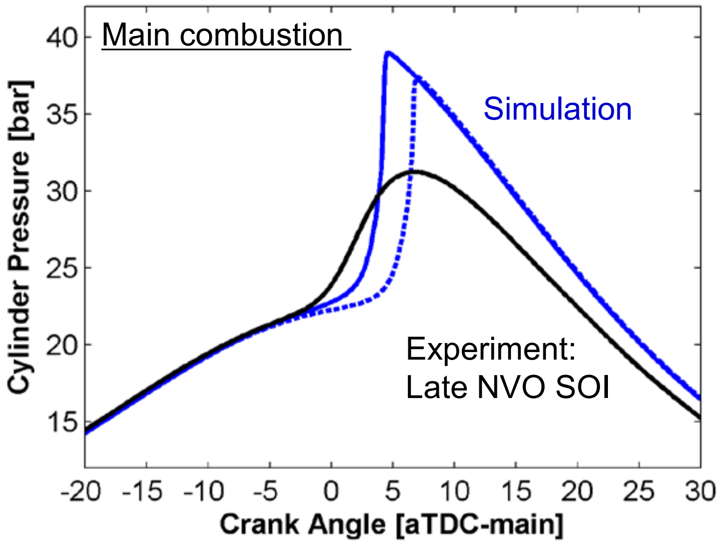
- Initial composition of simulation = major species plus the measured trace species shown in table.

» Adding second simulation enables an assessment of effect of trace species on CA50:
- Dashed line represents simulation using baseline initial composition, i.e. with none of the trace species.
- CA50 is significantly retarded, indicating that trace species are responsible for combustion enhancement.
- Further simulations reveal that C_2H_2 is the dominant species advancing CA50, with CH_2O showing a significant but reduced effect.



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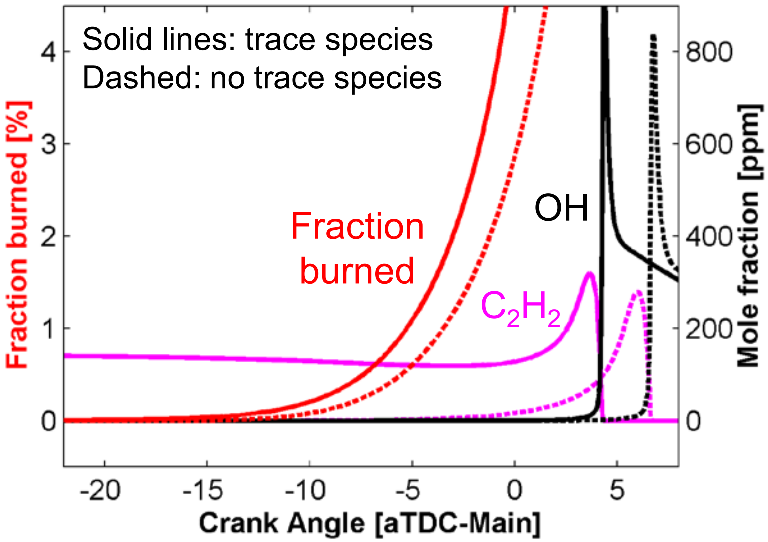
Simulations add to evidence of C_2H_2 combustion enhancement.

» Species profiles are displayed for the same pair of simulations.
  - The two OH profiles, which mark high-temp. reactions, quantify the phasing advance for late NVO injection.
  - Comparing fraction-burned and C_2H_2 curves indicates that the initial rise of the fraction-burned curve coincides with early consumption of C_2H_2 – further evidence of ignition enhancement.



» Significance of modeling results:
  - Chemkin predicts significant chemical effects of acetylene on main combustion in agreement with experiment.
  - These results increase confidence that the model can identify other reactive species of interest, contributing to knowledge of NVO chemistry.
  - Using a single-zone model allows simulation of homogeneous main combustion. Progressing to a multi-zone model will enable simulation of NVO reactions by capturing the inhomogeneous rich combustion associated with late injection.

Collaborations

»National Lab partners:

- Oak Ridge National Lab:
  - We both are conducting NVO sampling experiments:
    - Oak Ridge using a custom 6-stroke cycle, and
    - Sandia using the cylinder-dump technology.
  - We are collaborating on areas of overlap.
- Lawrence Livermore National Lab:
  - Currently providing chemical analysis expertise for engine sampling experiments.
  - Ongoing development and support for chemical kinetics models.
  - Development of KIVA model of our optical engine (with University of Wisconsin).

»Automotive OEM partners:

- GM Research: Extensive interactions include regularly scheduled teleconferences, exchange of technical results, hardware support, and active feedback on HCCI research directions.
- Ford Research: On-going interactions on topics of mutual interest.

»DOE Working Group partners:

- Research results are shared with DOE's Advanced Engine Combustion and University HCCI Working Groups that meet semi-annually.

Future Work

» Remainder of FY13

- Extend the range of operating conditions for NVO sampling experiments. Complete analysis and modeling. Assimilate results from parallel sampling experiments at ORNL.
- Initiate an investigation of advanced ignition technologies:
  - Determine the evolving ignition demands of lean- and dilute-combustion engines.
  - Identify innovative technologies that address these demands including cool plasma, microwave, laser, and spark-assisted compression ignition.

» FY14:

- Incorporate new ignition technologies into experiments focused on improving control of dilute and low-temperature combustion.
  - Probe fundamental ignition processes for selected technologies.
  - Apply technology to enhance HCCI-NVO and other combustion strategies.

Summary

» Our current work focuses on achieving combustion control using NVO. The strategy facilitates efficient and clean HCCI combustion for low-load operation in mixed-mode (SI-HCCI) engines.

» Progress this year includes:

- Completed study characterizing combustion enhancement effects of acetylene seeding.
- Fabricated a cylinder-dump sampling system to extract cylinder contents following NVO.
- Conducted sampling experiments using a sweep of NVO injection timings. We found that:
  - Concentrations of small hydrocarbons, including acetylene/ethylene, increase rapidly as NVO SOI approaches TDC.
  - Observations add to evidence from multiple earlier experiments that products from late NVO fueling can chemically enhance main combustion.
  - Chemkin simulations support the theory that acetylene is an important contributor to that enhancement.

» Clarifying the chemistry of NVO reactions enables optimization of NVO technology, thereby enhancing its contributions to engine efficiency and low emissions.