Automotive HCCI Engine Research

Richard Steeper
Sandia National Laboratories

2009 DOE Vehicle Technologies Annual Merit Review
Arlington, VA
May 18, 2009

Program Manager: Gurpreet Singh
DOE Office of Vehicle Technologies

Project ID: ace_06_steeper

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
• FY08 funding:
  – Sandia: $580k
  – Stanford: $115k
• FY09 funding:
  – Sandia: $580k
  – Stanford: $58k (ends June 2009)

Barriers identified in Light-Duty Roadmap
• Fundamentals of in-cylinder processes for LTC*
  – Fuel injection, evaporation, and mixing.
  – Heat transfer and thermal stratification.
  – Ignition, combustion, and emissions formation.
• Accurate simulation of in-cylinder processes
  – Fidelity of engine-combustion models needs to improve.
  – Simulations are needed to guide and interpret experiments.

Partners
• Project lead: Sandia - Richard Steeper
• Stanford University
  – Diagnostic development for HCCI labs (Steeper and Dec).
  – Includes Sandia hosting of students.
• LLNL and University of Wisconsin
  – CFD/kinetics model of automotive HCCI optical engine.
• Industry

* LTC: Low-temperature combustion
Objectives

- **Overall objective:** Expand our fundamental understanding of LTC in-cylinder processes to help remove barriers to the implementation of clean and fuel-efficient automotive HCCI engines.

- **Near-term objectives:**
  - Quantify thermal and chemical effects of negative valve overlap (NVO) strategy used to control and extend HCCI combustion.
  - Develop and apply diagnostics capable of quantifying in-cylinder NVO processes.
  - Facilitate model development. Validate and apply the models to interpret and supplement experimental data.
  - Plan facility upgrade to enhance optical access, extend operating range, and incorporate hardware common to industry research engines.
Milestones

• Complete benchmark experiments of NVO performance in metal and optical configurations of the automotive HCCI engine.

• Conduct experiments comparing NVO performance with and without NVO fueling for insight into the influence of reforming reactions on main combustion.

• Adapt Stanford 2-line planar laser-induce fluorescence (PLIF) diagnostic for application during NVO operation.

• Develop an optical diagnostic for CO measurement during re-expansion.

• Validate KIVA model of optical engine during motored NVO operation.
Approach

• Benchmark NVO low-load operation in metal and optical engines:
  – Gain insight into NVO fuel reforming by comparing performance with and without NVO fuel injection.

• Determine controlling NVO processes using optical diagnostics:
  – Continue Stanford-Sandia diagnostic development. Apply 2-line PLIF diagnostic to simultaneously map temperature and composition during fired NVO operation.
  – Develop a line-of-sight, IR absorption diagnostic to monitor species concentration during NVO reformation.

• Employ modeling tools to guide HCCI experiments and interpret results:
  – Apply models ranging from a 1-D full-engine simulation to a 3-D CFD simulation of in-cylinder flows and combustion.

• Interact with industry and other researchers to leverage research progress:
  – Address DOE- and industry-identified barriers and disseminate research results.
  – Adapt current industry hardware for our optical engine to enhance the relevance of our research.
FY09 Accomplishments

• Current work focuses on NVO engine operation as a promising strategy for HCCI combustion control at low-load conditions.

• Progress of our NVO research in FY09 is described in following slides, in this order:
  1. NVO engine experiments,
  2. Modeling development and application,
  3. Diagnostic development and application.

**Typical operating conditions**

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Valve overlap</td>
<td>-150 CAD</td>
</tr>
<tr>
<td>Resid. gas fraction</td>
<td>~50%</td>
</tr>
<tr>
<td>Geom. compr. ratio</td>
<td>11.5</td>
</tr>
<tr>
<td>Speed</td>
<td>1200 rpm</td>
</tr>
<tr>
<td>Fuel</td>
<td>Iso-octane</td>
</tr>
</tbody>
</table>
NVO benchmark experiments completed:

- We used split fuel injection, and varied 2 NVO parameters:
  - NVO fuel percent sweep:
    - At low NVO fueling, CA50* is very sensitive to fuel percentage.
    - Effect disappears at higher fuel percent due to insufficient oxygen for complete reaction during NVO.
  - NVO start of injection (SOI) sweep:
    - For early SOI, retarding injection decreases NVO IMEP and advances CA50.
    - For late SOI, trends change due to reduced time for reactions and increased piston wetting.
    - Why does decreasing NVO HR advance CA50?
- Conclusion: NVO fueling effects depend on multiple factors:
  - NVO heat release
  - NVO heat-release phasing
  - Unreacted NVO fuel
  - Reformed NVO fuel

* CA50: Location of 50% heat release (HR) of main combustion
We have fulfilled an industry request to compare NVO operation with and without NVO fuel injection:

• Goal is to assess the relative importance of NVO chemical and thermal effects on main comb. phasing.

• Experiment setup: split-injection vs. main-injection
  – Phasing of split-injection experiments is controlled using either NVO SOI or NVO fuel percent.
  – For the main-injection experiments, we hold main fuel mass constant, and then vary (increase) intake temperature to achieve normal phasing.
  – The split-injection case potentially includes both thermal and chemical influences on CA10, while in the main-injection case, thermal effects are the only influence.
  – Comparing the two thus yields a measure of the chemical effect of NVO fueling on main combustion.

• To facilitate comparison of these data, we developed a model for estimating cycle temperatures, as explained in the next slide…
A cycle-temperature model has been developed for comparing NVO engine experiments:

- Temperature calculations are based on known mass, pressure, and volume plus measured reference temperatures (intake and exhaust).

- Pegging the closed portions of the cycle to the reference temperatures is done using:
  - GT Power engine model.
  - CHEMKIN ignition temperature estimates.

- Calculations have also been compared to PLIF measurements of in-cylinder temperatures:
  - Measurements were made using Stanford diagnostic described later.
  - Agreement is good, but still working on tuning.

- Using the temperature calculations for comparison of the split- vs. main-injection experiments is demonstrated in the following slide…
Split- vs. main-injection experiments have provided insight into the effects of NVO fuel injection:

- In the bottom graph, temperatures calculated at intake valve closing (IVC) are plotted against CA10:
  - For the main-injection case, control parameter is $T_{\text{INTAKE}}$: as it is increased, $T_{\text{IVC}}$ increases, and phasing advances.
  - For the split-injection case, as NVO fuel % is increased, $T_{\text{IVC}}$ increases, and phasing advances.

- Comparing the curves provides insights:
  - Temperatures of the two cases are close, meaning that NVO fueling has provided about the same thermal energy as heating the intake air.
  - Yet there is a distinct temperature difference, suggesting that some chemical effect makes up the difference.

- For further evidence, we can examine temperatures later in the compression stroke:
  - At 70 bTDC, the two cases have moved closer together.
  - Since compressive heating spreads all temperatures farther apart, some other effect is in play.
  - At 15 bTDC, split-fuel temperatures continue to rise.

- Knowledge gained:
  - For NVO fueling, we conclude that exothermic reactions occur during mid-compression, driving up temperatures.
A large number of the split- vs. main-injection experiments have been completed.

- Analysis of the results has provided a range of insights about chemical effects of NVO fuel addition:
  - In NVO SOI sweep experiments, observed effects are more complex than for the fuel % sweep (previous slide): For example, separate trends are seen for early vs. late NVO injection.
  - In another series of experiments, fuel was seeded with LIF tracer (to test potential interference by the tracer). In this case, we observe evidence of early endothermic reactions that suppress temperatures during compression.

- Our accumulated experimental observations emphasize the complex influence of NVO fueling on HCCI combustion.

- To help unravel these effects, we depend on our CFD/kinetics code.

- Next slide describes the CFD/kinetics code plus other modeling tools…
3-D KIVA/kinetics model of our optical engine is now capable of simulating fired NVO operation.

- Collaborative project with UW (KIVA) and LLNL (multi-zone kinetics) continues to make progress:
  - Motored NVO simulations have been validated.
  - We are currently validating fired NVO simulations against pressure, temperature, and emissions measurements.
    - Graph at right shows good experiment/simulation agreement.
    - Image at lower right shows sample time/temperature details of the NVO period.
  - Model results were published in an SAE journal article.

- We have developed a GT Power 1-D model of our engine to estimate flows and temperatures:
  - Provides boundary conditions for KIVA model as well as a consistency check on KIVA predictions;
  - Assists analysis of cycle temperatures.
  - Guides selection of experimental conditions.

- As described earlier, we have created a cycle-temperature model that facilitates our analysis of NVO operation.
Diagnostic development 1: Applying the 2-line PLIF diagnostic in our NVO engine

- Our joint project with Stanford has created an LIF diagnostic for simultaneous composition and temperature imaging.
- Details of the system were presented last year.
- Progress this year includes:
  1. Adapting the diagnostic for measurements during NVO recompression and re-expansion (next 2 slides).
  2. Measuring temperatures during fired NVO operation for a range of operating conditions. (Use of these data to validate our cycle-temperature model was discussed earlier.)
  3. Quantifying potential interference of LIF tracers on HCCI combustion (discussed later).
  4. Documenting details of the diagnostic and its application in three journal articles.
We have adapted the diagnostic to capture images during both the main and NVO portions of the cycle:

- Successful PLIF imaging requires:
  - Ability to get tracer into the cylinder and field of view (FOV) prior to imaging;
  - Avoidance of temperatures that decompose tracer;
  - Absence of droplets and interfering fluorescent species.

- We have made successful measurements during:
  - Main compression:
    - Tracer is premixed in intake air or injected with fuel.
    - Relatively little interference from non-tracer molecules.
    - Tracer coverage is good due to long mixing times.
  - NVO recompression:
    - Tracer is injected along with NVO fuel;
    - But short mixing time between injection and imaging means that tracer does not cover the full FOV.
  - NVO re-expansion:
    - Tracer injected during recompression has reacted by this time.
    - But we discovered that main injection can be advanced enough to enable imaging, as described in the next slide…
A method to enable PLIF measurements during NVO re-expansion has been devised:

- We use early main injection to make measurement possible:
  - Data are desired at the end of NVO, so image capture timing is set just before IVO.
  - To provide LIF tracer, main injection must be timed before imaging: Early enough for evaporation, but not so early that high re-expansion temperatures cause tracer decomposition.

- Sample single-cycle image pair at left demonstrates results:
  - The limited time between injection and image capture means limited fuel/tracer mixing, and only partial coverage of the field of view.
  - But in areas where there is sufficient tracer, temperatures are successfully mapped.
  - Note that stratification in the temperature image includes effects of evaporative cooling, but sufficient information is contained in the pair of images to separate these effects.

- This work shows that PLIF imaging can be applied during NVO, but an important issue remains: what is the possible impact of LIF tracers on combustion?
We have completed a detailed quantification of the effects of LIF tracers on HCCI combustion:

• LIF diagnostics typically rely on fluorescent tracers added to fuel or air flows:
  – The tracers can represent a significant fraction of the fuel caloric content.
  – In the case of commonly used ketones, the tracers are not normal fuel constituents.
  – As a result, the LIF tracers could potentially influence the combustion.

• We conducted a series of experiments to measure tracer impact, using:
  – Both single-stage and two-stage-ignition fuels: iso-octane and n-heptane.
  – Two common ketone tracers: acetone and 3-pentanone.

• Tests uncovered multiple trends, as illustrated in next two slides…
We measured and modeled the effects of seeding iso-octane with 3-pentanone and acetone:

- 3-Pentanone tracer advances the main combustion phasing of iso-octane.
- CHEMKIN engine simulator captures the trend well (although the single-zone model means combustion duration is artificially short).
- Acetone has the opposite effect, retarding main combustion.
- Again, CHEMKIN model corroborates the trend.
The experiments also characterized tracer seeding of n-heptane fuel:

- For the 2-stage fuel n-heptane, we found that both tracers retard combustion phasing:
  - Top graph shows 3-pentanone results, but phasing retard is similar for acetone.
  - Both low- and high-temperature reactions are retarded.

- But most importantly, we also found that it is easy to compensate for tracer effects via intake temperature:
  - Bottom graph shows that an intake temperature increase of 10 K re-establishes the original main-combustion phasing (acetone shown here).
  - Compensation for iso-octane + tracers requires smaller ΔT.

- Knowledge gained from the study:
  - Effect of LIF tracers on HCCI combustion is not trivial.
  - However, the magnitude of the effects is small enough to allow compensation by modifying inlet temperatures.
  - Details are documented in an SAE journal article.
Diagnostic development 2: We have designed and are testing an IR-absorption monitor for NVO use:

- Decoding fuel reformation is a key to successfully developing NVO:
  - Temperature measurements and analysis discussed earlier provide part of the picture;
  - But composition measurements are crucial to mapping NVO reforming reactions.
  - CO is an obvious marker of reaction progress, and a good candidate for optical detection.

- To address the need, we built a simple, IR-absorption diagnostic for CO detection:
  - Near-IR, tunable diode laser light is delivered by fiber and detected at 2x modulation frequency for improved SNR.
  - Multi-pass, line-of-sight design provides time-resolved, spatially averaged measurements.
  - The goal is sufficient sensitivity to record in-cylinder CO concentrations during NVO re-expansion with crank-angle resolution.
Bench test results are positive:

- Sensitivity achieved to date is sufficient (but not yet maximized):
  - Using 6 passes, we currently capture sufficient signal to detect CO as low as 4000 ppm (graph at left).
  - Expected end-of-NVO concentrations are 5k – 15k ppm.

- Setup of bench tests will make switch to engine easy:
  - Identical geometry allows bench-optimization of sensitive optical alignment.

- The diagnostic is nearly ready for engine testing, and following that, we will have a new tool to advance our analysis of NVO performance.
Future Work

• Measure the variation in end-of-NVO concentration of CO during NVO parameter sweeps using absorption diagnostic. Determine correlation of CO concentration with NVO fuel, cycle temperatures, and combustion performance.

• Measure the performance effect of seeding intake air with CO during main-injection experiments for further insight into chemical effects of NVO fuel injection.

• Complete validation of KIVA model for fired NVO operation. Run the code at conditions of the split- vs. main-injection experiments to identify controlling reactions and species during NVO reforming.

• Improve sensitivity of CO diagnostic to allow calibration using engine exhaust at concentrations near 1000 ppm.

• Upgrade engine facility:
  – Plan modifications to benefit from the design and installation of similar engine hardware in a new Lean-Burn DI Spark-Ignition Fuels Lab (Sjöberg).
  – End results will improve optical access, extend operating conditions, and more closely duplicate current industry hardware.
Summary

• The Automotive HCCI Engine project contributes to the development of low-temperature combustion strategies that provide a path to achieving national emissions and efficiency goals.

• The project approach combines:
  – Optical engine experiments,
  – Diagnostic development,
  – Engine and combustion modeling.

• Work this year focused on the NVO combustion strategy. Accomplishments included:
  – Parametric NVO fueling experiments,
  – PLIF measurements,
  – CO diagnostic development,
  – Model validation.

• Multiple collaborations leverage the impact of our research:
  – DOE’s Advanced Engine Combustion group reviews research results and contributes feedback;
  – Industry partners provide engine hardware and frequent guidance;
  – Stanford, University of Wisconsin, and LLNL participate in the project.

• Next year we will continue our efforts to sort out the effects of NVO fueling on HCCI combustion.