Low Temperature Automotive Diesel Combustion

Light-Duty Combustion Experiments
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Light-Duty Combustion Modeling
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Project ID# ACE002
Overview

Timeline:
- Project has supported DOE/industry advanced engine development projects since 1997
- Direction and continuation evaluated yearly

Barriers addressed:
- A Lack of fundamental knowledge
- B, G Lack of cost-effective emission control
- C Lack of modeling capability

Technical targets addressed:
- 40% diesel fuel economy improvement
- Tier 2, bin 2 emissions
- Emission control efficiency penalty < 1%
- 30 $/kW power specific cost

Budget:
DOE funded on a year-by-year basis
- SNL $730k (FY11), $725k (FY10)
- UW $230k (FY11), $230k (FY10)

Partners:
- 20 industry/national laboratory partners in the Advanced Engine Combustion MOU
- Close collaboration with GM-funded research at UW (Foster)
- Additional post-doc funded by GM
Relevance of Sandia’s major technical accomplishments (May 2010 – March 2011)

1. Varied ignition quality and volatility independently in an orthogonal matrix to examine the impact of these fuel properties on LTC CO and UHC emissions
   Barriers/Targets: Improved fundamental understanding of the role of fuel properties on enabling LTC combustion; fuel property parameter sweeps for modeling validation & sensitivity studies; Tier 2, bin 2 emissions target; 40% diesel fuel economy improvement (links to UW 1)

2. Assessed accuracy and implementation of RNG turbulence models
   Barriers/Targets: Improved modeling of in-cylinder processes (UW 2)

3. Examined asymmetries and mean flow structure in the induction flow via Particle Image Velocimetry
   Barriers/Targets: Improved understanding and improved modeling of in-cylinder processes (UW 3)

4. Investigated wall-wetting by post-injections for PM trap regeneration for various injection timings and diesel/biodiesel fuel blends
   Barriers/Targets: Improved understanding of in-cylinder processes (penetration, spray disruption by exhaust flows); efficiency penalty of PM trap regeneration; 30 $/kW cost target

5. Consolidated measurements and simulations to provide a phenomenological picture of light-load LTC combustion
   Barriers/Targets: Improved understanding and improved modeling of in-cylinder processes; Tier 2, bin 2 emissions target; 40% diesel fuel economy improvement (links to past UW work)
Relevance of UW’s major technical accomplishments (May 2010 – March 2011)

1. Examined sources of discrepancy in UHC and CO distributions between model and experiment & identified spray/entrainment model as a dominant source
   Barriers/Targets: Improved understanding and improved modeling of in-cylinder processes; Tier 2, bin 2 emissions target; 40% diesel fuel economy improvement (links to SNL 1)

2. Evaluated variable density gas jets and engine flows with RNG turbulence closure; derived alternative model dependent on the ‘dimensionality’ of the strain
   Barriers/Targets: Improved modeling of in-cylinder processes (SNL 2)

3. Examined intake flow modeling with detailed port, valve, and combustion chamber mesh; examine impact of flow-field non-uniformities on UHC and CO
   Barriers/Targets: Improved understanding and improved modeling of in-cylinder processes; Tier 2, bin 2 emissions target; 40% diesel fuel economy improvement (SNL 3)

4. Examined light-duty RCCI combustion; upgraded engine fuel system(s)
   Barriers/Targets: Improved understanding and improved modeling of in-cylinder processes; Tier 2, bin 2 emissions target; 40% diesel fuel economy improvements

5. Improved soot model based on PAH kinetics; compared results to conventional, PCCI, and RCCI combustion in light- and heavy-duty engines
   Barriers/Targets: Improved understanding and improved modeling of in-cylinder processes; Tier 2, bin 2 emissions target; 40% diesel fuel economy improvement; cost-effective emission control
Our approach coordinates and leverages the strengths of several institutions and funding sources:

**Technical/Programmatic Approach**

### Programmatic:
- Multi-institution effort focused on a single hardware platform
- Significant leverage of DOE funds by support from other sources

### Technical:
- Closely coordinated program with both modeling and experiments
- Input from and technical transfer to industry inherent in program structure
Accomplishments: In-cylinder sources of UHC/CO

Task:
Investigate the impact of fuel ignition quality and volatility on the UHC/CO emissions and combustion efficiency of PCI LTC through measurements made in an orthogonal fuel property matrix.

Results:
Cetane number is the dominant fuel property impacting UHC & CO.

Large volatility changes are needed to impact engine emissions.

Images show that despite greater piston films and crevice UHC, low volatility fuels provide lower bulk gas UHC & CO.

High ignition quality likewise lowers bulk gas UHC & CO.

Variation in bulk gas CO as cetane number varies with fixed volatility (UHC is similar).
Task:
Identify the source of the discrepancy between the experiments and regarding the dominant in-cylinder source of UHC and CO emissions

Results:

Previous work demonstrated that:
- Improvements to reduced kinetic mechanism helped, but did not fully resolve the discrepancy
- Investigated sensitivity to $T_{in}$, grid resolution, $O_2$, bowl volume, $C_d$
- Remaining discrepancy associated with mixing processes

This year have investigated model sensitivity to:
- $R_s$, "swipro", $P_{inj}$, $T_{wall}$, SOI, $m_{fuel}$, turb. & wall impingement models

Results have the greatest sensitivity to $R_s$ and $P_{inj}$

But the most promising improvement was associated with the new gas jet spray modeling:

Future work will focus on model tuning to predict a range of $R_s$, $P_{inj}$, and $d_{nozzle}$
Accomplishments: Turbulence model assessment

The flow and turbulence modeling underpins the simulation of the mixing and combustion processes.

Background:
Standard k-ε turbulence modeling cannot predict both compression and expansion with a single set of constants.

Task:
Investigate the performance of the (variable constant) RNG k-ε model.

Results:
The RNG closure severely overestimates k and ℓ, due to the underestimation of ε.

The penetration of variable density gas jets is underpredicted for the same reasons.
Accomplishments: Turbulence model shortcomings: causes and redress

KIVA RNG $k$-$\varepsilon$ coding:

\[
C_3 = \frac{-4 + 2C_1}{3} + \frac{1}{(\nabla \cdot \mathbf{U}) v} \frac{1}{dt} \left[ \frac{1}{3} - \frac{\sqrt{6}}{3} \frac{\eta^2 (1 - \eta/\eta_0)}{1 + \beta \eta^3} (\varepsilon - 1) \right]
\]

As implemented, $C_3$ is computed as strain rate ($S_{ij}$) dependent – it is not evaluated in the rapid distortion limit.

In this case, the RNG-specific terms are:

\[
\mathcal{R}_t + C_{3, \eta} \varepsilon (\nabla \cdot \mathbf{U}) = \frac{C_\mu \eta^2 (1 - \eta/\eta_0) \varepsilon}{1 + \beta \eta^3} \left[ \sqrt{2S_{ij}S_{ij}} - \frac{\sqrt{6}}{3} \left| \nabla \cdot \mathbf{U} \right| \right]
\]

Difference between the characteristic strain rate and the characteristic rate associated with pure spherical distortion, $S_{11} = S_{22} = S_{33} = (\nabla \cdot \mathbf{U})/3$

Redress:

An alternative compressible RNG closure based on the ‘dimensionality’ of the flow field has been developed and is being tested.

Future work will focus on more thorough model testing against engine measurements and DNS calculations.
**Accomplishments:**

**In-cylinder flow characterization**

**Task:**
Characterize in-cylinder flow structure to:

i) Validate induction stroke calculations

ii) Clarify flow structure for closed-cycle simulations

iii) Evaluate asymmetry of the pre-combustion flow (need for 360° grid)

**Method:**
Horizontal Plane PIV with distortion correction

**Results:**

- **50° b TDC**
- Black circle identifies center of swirl structure
- Numbers in parenthesis represent swirl ratio, circles represent 1-σ deviation
- Swirl center tilt (and precessional motion) is:
  - Insensitive to swirl ratio
  - Present in individual cycles
  - Less variable at high $R_s$

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Symbols:
- $h = 3\,\text{mm}$
- $h = 10\,\text{mm}$
- $h = 18\,\text{mm}$

Images:
- Raw Image
- Corrected Image

**Laser Sheet**

**Piston Mirror**

**Exhaust**

**Intake**

**30 m/s**
Accomplishments: In-cylinder flow characterization

Results:

- $\alpha = 2.3$, $R_s = 2.1$

The average value of $\alpha$ ("swipro") over all swirl ratios and measurement locations is $\bar{\alpha} = 2.2$

Comparison with previous LDV data suggests this value is independent of port geometry.

Comparison with model results:

A full 3-d mesh of the GM engine has been created.

Comparison with horizontal and vertical plane PIV measurements, for various turbulence models, is in progress (Note the absence of a major clearance volume vortex)

$$V_\theta(r,t) = \frac{\omega_c r_b R_x \alpha}{4 J_2(\alpha)} \cdot J_1\left(\alpha \frac{r}{r_b}\right)$$
Accomplishments: Post-injection wall wetting with biofuel blends

Task:
Examine the impact of biodiesel content on wall-wetting when post-injections for DPF regeneration are employed
i) Neat D2 versus biofuel blends
ii) Impact of injection timing
iii) Potential for jet disruption by exhaust flows

Results:
With early post-injection, none of the fuels wet the cylinder wall (consistent with liner friction studies)

All of the fuels impact the cylinder wall with conventional timing, even with small post-injection quantities. Wetting is more severe and persistent with biofuel blends.

Injection during the exhaust blowdown period fails to significantly disrupt jet penetration.

Method:
Simulate in cylinder conditions typical of highway-like PDF regeneration (5 bar, 1500 rpm) assuming a close coupled DOC.
Accomplishments: Data consolidation and phenomenological picture of light-duty LTC

Heavy-duty LTC (Musculus & Pickett)

Light-duty, early-injection LTC

Intermediate Ignition (CO, UHC)
Second-Stage Ignition of Intermediate Stoichiometry or Diffusion Flame (OH)
Liquid Fuel
First-Stage Ignition (H₂CO, H₂O₂, CO, UHC)
Pre-ignition Vapor Fuel
Head of Entrainment Wave
Soot or Soot Precursors (PAH)
Collaborations

Within Vehicle Technologies program:

- Formal collaboration between SNL-UW-ORNL
- Participation in Advanced Engine Combustion group, including presentations and discussion with 20 industrial/national laboratory partners:

Ex-Vehicle Technologies program:

- Close ties with GM:
  - GM-funded post-doctoral researcher
  - Monthly teleconferences (Diesel and LES working groups)

- Strong ties to Lund University:
  - Exchange students perform research at Sandia
  - SNL staff participates in LU research projects
Future work – SNL/UW

- Examine the impact of various engine design and operating parameters on in-cylinder sources of UHC and CO:
  - Swirl ratio, injection pressure, hole size
  - Multiple injections

  Demonstrate/develop a predictive modeling capability

- Measure pre-combustion equivalence ratio distributions to aid in model validation and interpretation of UHC/CO data

- Continue work on validating or developing new RANS-based turbulence models to enable more accurate dissipation modeling (compare to existing / new high-Re DNS calculations – Joe Oefelein)

- Investigate the impact of flow and geometric asymmetries on combustion and emission formation (Extend PIV measurements to squish volume near TDC, horizontal plane UHC imaging near TDC

  Demonstrate develop capability to quantitatively predict flow structures, including asymmetries
Summary

- **Project focuses on several barriers/targets identified in the EERE-VT program plan:**
  - Lack of fundamental knowledge
  - Lack of modeling capability
  - 30$/kW specific cost; Tier 2, Bin 2 emissions
  - Lack of cost effective emission controls
  - Emission control efficiency penalty
  - 40% diesel fuel economy improvement

- **Technical accomplishments this reporting period include:**
  - Understanding of the impact of fuel properties on LTC UHC/CO in-cylinder emission sources
  - Improved modeling of LTC combustion and UHC/CO emissions
  - Identification of problems with compressible RNG turbulence model and implementations
  - New compressible RNG closure model dependent on mean flow ‘dimensionality’
  - Measurement of swirl flow structure and asymmetries; full 360° grid and initial simulations
  - Imaging study of post-injections spray wall impingement for neat diesel and biofuels
  - Consolidation of data and development of phenomenological picture of light-duty LTC to complement heavy-duty work

- **Future work will include:**
  - Continuation of UHC/CO imaging and modeling, with emphasis on capturing the influence of engine design and operating parameter dependence; measurement of pre-combustion $\phi$-dist.
  - Continued efforts to improve compressible RANS flow modeling – which underpins the modeling
  - Continuation of flow (and horizontal plane UHC distributions), with an emphasis on understanding asymmetries and the necessity of modeling them