

#### ACE001: Heavy-Duty Low-Temperature and Diesel Combustion & Heavy-Duty Combustion Modeling

Mark P. B. Musculus Combustion Research Facility

#### Sandia National Laboratories

FY 2010 DOE Vehicle Technologies Program Annual Merit Review Advanced Combustion Engine R&D/Combustion Research 8:30 – 9:00 AM, Tuesday, May 15, 2012



Sponsor: U.S. Dept. of Energy, Office of Vehicle Technologies Program Manager: Gurpreet Singh ACE001

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#### Heavy-duty combustion project overview

### Timeline

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

### Budget

 Project funded by DOE/VT: FY11-SNL/UW: \$700/115K FY12-SNL/UW: \$700/115K

### Barriers

- Inadequate understanding of fuel injection, mixing, thermodynamic combustion losses, combustion/ emission formation processes
- Inadequate capability to accurately simulate these processes.

### Partners

- University of Wisconsin, Delphi
- 15 industry partners in the AEC MOU
- Project lead: Sandia (Musculus)





#### **Long-Term Objective**

Develop improved understanding of in-cylinder LTC spray, combustion, and pollutant-formation processes required by industry to build cleaner, more efficient, heavy-duty engines

Current Specific Objectives:

- ① SNL Distill observations spanning years of optical and computational research into conceptual model for LTC
- ② SNL Implement and demonstrate new high precision fuel system for multiple injections in optical engine
- ③ SNL Explore close-coupled post injections for mitigating PM emissions and improving fuel efficiency
- **4** UW Compare the multi-mode model predictions to exp. data and identify directions for improving thermal efficiency





- 1. (SNL) Demonstrate new common-rail fuel injection system for controlled multiple injections.
- 2. (SNL) Evaluate small post injections for mitigating pollutant emissions and improving fuel efficiency
- 3. (UW) Compare multi-mode combustion model predictions to measurements of combustion propagation from FY 2011
- 4. (UW) Compare the multi-mode combustion model predictions to experimental data spanning conventional diesel to advanced LTC combustion taken, and identify directions for thermal efficiency improvements



#### Approach: optical imaging and CFD modeling of *RE* in-cylinder chemical and physical processes

- Combine planar laser-imaging diagnostics in an optical heavy-duty engine with multi-dimensional computer modeling (KIVA) to understand LTC combustion
- Transfer fundamental understanding to industry through working group meetings, individual correspondence, and publications







- All work has been conducted under the Advanced Engine Combustion Working Group in cooperation with industrial partners
  - Cummins, Caterpillar, DDC, Mack Trucks, John Deere, GE, International, Ford, GM, Daimler-Chrysler, ExxonMobil, ConocoPhillips, Shell, Chevron, BP, SNL, LANL, LLNL, ANL, ORNL, U. Wisconsin
- New research findings are presented at biannual meetings
- Tasks and work priorities are established in close cooperation with industrial partners
  - Both general directions and specific issues (e.g., UHC for LTC, soot in higher load conditions)
- Industrial partners provide equipment and support for laboratory activities
  - FY2012: Delphi provided new injection system with support





 Accomplishments for each of the four current specific objectives below are described in the following fourteen slides

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### Sandia's conceptual model for conventional diesel is cornerstone of understanding

 Sandia's conceptual model of diesel combustion was developed based on observations from multiple laser/imaging diagnostics over many years of optical engine research



With many years of LTC optical engine research under our belt, can we develop a conceptual model for diesel LTC?

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#### 1 LTC spray penetrates more quickly + longer liquid; liquid recedes after EOI, before SOC

- Injection into lower density: faster spray penetration, longer liquid length
- Liquid recedes before SOC as vapor hits piston wall





### 1-D analytic, KIVA RANS, and Sandia LES models predict wave of increased entrainment after EOI

Head of Entrainment

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Wave

- Reduction in upstream jet velocity draws in more entrainment, which reduces velocity further, driving more entrainment, etc.
- LES (Oefelein, Hu): EOI ramp-down causes large flow structures to separate rather than collide; ambient fluid is entrained into gaps 5.0°



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#### First-stage ignition in downstream vapor fuel, partially burned fuel (UHC, CO) throughout jet

- LLNL chemical kinetics model: formaldehyde at 1<sup>st</sup>-stage ignition
- Experiments: Formaldehyde fluorescence at 1<sup>st</sup> stage, throughout jet



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### Second-stage ignition downstream where $\phi$ ~1, followed by soot in rich pockets at head of jet

First-Stage Ignition

Intermediate Ignition

(H<sub>2</sub>CO, CO, UHC)

2nd-Stage Ignition

or Diff. Flame (OH)

(CO, UHC)

10.0°

ASI

Second-Stage

gnition of fuel-

rich mixtures

Soot or Soot

Precursors (PAH)

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- Soot and PAH form in  $\phi$ >2 pockets
- In lean upstream regions, experiments and LLNL kinetics simulations show partially burned fuel (CO, UHC, formaldehyde) ——



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#### Late cycle: soot pockets largely oxidize, formaldehyde, CO, UHC remain upstream



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### Experiments show over-lean regions near injector, where kinetics models predict partial combustion

- Experiments: vapor-fuel tracer-PLIF shows lean mixtures near injector where combustion-PLIF shows late-cycle formaldehyde and CO
- LLNL kinetics models: Lean mixtures have long dwell between first- and Distance from Injector [mm] 5 AEI 0 AEI second-stage ignition, with UHC and CO persisting to exhaust Distance from Injector [mm]  $\phi$  from **Kinetics Model** 1 AEI experiment 0.6 0.06 0.8 Timing retard shifts mixture Distance ... Injector [mm] 0.05 distribution toward leaner  $\phi$ Mole fraction CO, UHC 2 AEI 0.04 UHC 0.03 Distance from Injector [mm] The threshold for 0.02 lean-mixture 3 AE 36 AEI oxidation increases as timing is retarded 0.01 L> 20 10 20 30 40 10 30 40 0.2 0.4 0.8 1.2 1.4 Distance from Injector [mm] Distance from Injector [mm] 0 0.6 1 1.6 Equivalence Ratio,  $\phi$



#### 1 LTC conceptual model review article includes both heavy- and light-duty perspectives

Early-injection LTC

20 30 40 mm

-22° 0

-20° 3° ASI

1° ASI

Late-injection LTC

2.25° ¢

4.25° 4

3° ASI

Peak

1° ASI

20 30 40 mm

Peak

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- Team effort with Lyle Pickett and Paul Miles
- March 2012: LTC conceptual model in review (PECS), publication pending



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#### New fuel injector/system implemented for new effort requiring precise multiple injections

- Optical cylinder head modified to accept Delphi DFI-1.5 injector
- New 0.2 liter accumulator (rail) close to injector to minimize rail dynamic effects
- Delivers close-coupled post-injections down to ~1-2 mg with IMEP COV <1%</li>
- This injector is first step; may follow with other injectors (e.g., direct piezo, fast heavy-duty)





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# CRF 3

# PM reduced by close-coupled post injections for wide range of EGR, + good combustion phasing

- Previous work with LTC postinjections showed a benefit only at late timings
  - Soot-free post injection oxidized main-injection soot, but only in squish
  - Significant efficiency penalty for late injections
- New injector shows benefit for close-coupled post injections
  - Similar effect realized at 21%, 18%, 15% and 12% intake O<sub>2</sub>
  - Minimum-PM post-injection (7-15 mg) adds 50-100 kPa IMEP
  - Post-injection is close-coupled, so combustion phasing is favorable for efficiency



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#### Initial results shows how interaction between main and post injections needs proper post penetration

- Small post-injection
  - Luminous soot from post-jet penetrates only half of piston-bowl radius
  - Exhaust soot is similar to main-injection only, implying little interaction between injections
- Larger post-injection
  - Post-jet penetrates across bowl and impinges on bowl-wall
  - Post injection helps to oxidize main injection soot within bowl

### Interaction details to be probed with laser diag.



(click movies to play)

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# CRF. 4

### CFD for RCCI predicts early flame propagation, but effects on global heat release is small

- FY11 laser-ignition experiments showed potential for flame propagation in dual-fuel (gasoline+diesel) Reactivity-Controlled Compression Ignition (RCCI) combustion (e.g., near piston bowl)
- Using a G-equation model with Damköhler number criterion predicts many cells initially dominated by flame propagation
- Predicted heat release similar to no flame propagation model



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# Global combustion characteristics captured by single UW-Kiva code across wide mode range

- Model cylinder pressure agrees with multi-mode experiments
  - Conventional high-temperature diesel combustion with short ignition delay (HTC-Short)
  - Low-temperature diesel combustion with long ignition delay (LTC-Long)

10

0

Crank [°ATDC]

- Dual-fuel RCCI combustion

Experiment

Simulation

-10



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-30

-20

6

Pressure [MPa]

### CRF. 4

# Simulations point to heat transfer & combustion design for further efficiency improvements



- Model energy balance analysis shows RCCI efficiency improvements are primarily due to reductions in heat transfer
- Heat transfer is reduced by lowering peak temperature
  - Highly premixed operation results in peak equivalence ratio near 0.5
  - Additional temperature reductions are due to EGR
- Further reductions in heat transfer are achieved by keeping high-temperature regions away from surfaces



# Future Plans: Build multi-injection conceptual model, heat transfer diag., and LTC PAH/soot

- Start building a design-level conceptual-model understanding of multiple injection processes
  - Explore fuel-injection schedules using multiple pilot, post, and split injections that are currently deployed by industry
  - Identify mechanisms and critical requirements (injector rate-shaping, dwell, duration, etc.) to achieve emissions and efficiency improvements across wide parameter space
- Determine how combustion design affects heat transfer and efficiency
  - Measure spatial and temporal evolution of heat transfer across range of combustion modes; correlate to progression of in-cylinder combustion processes
- Build understanding of in-cylinder LTC soot and PAH
  - Use multiple laser wavelengths and high-temporal-resolution imaging/spectroscopy to track PAH growth and conversion to soot



### **RE** Heavy-Duty Combustion and Modeling Summary

Improved understanding of in-cylinder LTC spray, combustion, and pollutant-formation to help industry build cleaner, more efficient engines



(SNL) Distilled recent years of optical LTC research into conceptual model for both heavy- and light-duty



(SNL) New injector and delivery system provides repeatable, precise close-coupled multiple injections



(SNL) Close-coupled post-injections reduce soot over range of EGR; images show multi-injection interactions



(UW) Model predictions show efficiency is improved by combustion design to reduce heat transfer

