Applied Computational Methods for New Propulsion Materials

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### ProjectOverview

#### Timeline
- Project start – Q3 FY2014
- Project end – Q4 FY2019
- Ongoing

#### Barriers
- **Directly targets barriers identified in VTO MYPP**
  - “Changing internal combustion engine combustion regimes”
  - “Long lead times for materials commercialization”
  - “Many advanced vehicle technologies rely on materials with limited domestic supplies”
  - “Need to reduce the weight in advanced technology vehicles”

#### Budget
- FY2017 – $235 K
- FY2018 – $230 K
- FY2019 – $210 K

#### Partners
- Convergent Science, Inc.
- Two engine OEMs
Power-density trends in HD engines present challenges for materials with higher temperatures and pressures

- **Trend**: Roadmap for heavy-duty (HD) engine operation projects increasing specific output, with **higher peak cylinder pressures (PCP)** and **temperatures** into the foreseeable future
- SuperTruck I programs showed >50% BTE with ≈225 bar PCP, for short timespans

- **Challenge**: Materials properties degrade with temperature
  - Concerns: Strength, creep, fatigue, oxidation/corrosion, cost

Many cast irons have similar tensile properties at elevated temperatures, but creep and fatigue life are also important. Additional materials properties, including fatigue life, determine suitability for more intensive engine applications.
Gas-materials interface is important in engine modeling, analysis, and operation

- Cylinder walls contain combustion gases, provide heat-transfer interface
- Extreme environment has impact on materials (e.g., corrosion, stresses)
- Spatially varying heat flux is important in evaluating materials stresses
- Traditional combustion modeling uses specified boundary conditions
- Advances in simulation now support temperature predictions and more accurate heat-flux co-solution of gases and structural solids [this project]

In the diagram:

- **COOLANT** boundary
- **HEAD** cylinder walls
- **PISTON** area

Temperature and heat transfer symbols:
- **T** : temperature
- **P** : pressure
- **Q** : heat transfer

**Cylinder boundaries**

**Stress map in engine head**

Injector removed (lower resultant stresses)
EV: Exhaust valve
IV: Intake Valve

**RELEVANCE**
This project integrates experiment and modeling.

**DESIGN**
Increase in specific power → higher cylinder pressures & temperatures

**EXPERIMENT**

1. **Compacted Graphite Iron**
   - Thermo-mechanical properties
   - Fatigue, creep

2. **GT-POWER**

3. **Low-order model**

4. **Finite Element Model**
   - Temperature, stress, strain maps

5. **Fatigue models at power-dense conditions**

**WORKFLOW FOR MATERIALS PROPERTIES TARGETS**

**CONVERGE**

- Combustion models (CFD)
- Heat flux maps
- Parametric studies (fixed, estimated temperatures)
- Conjugate Heat Transfer (solved temperatures, accurate heat-flux spatial maps)

**APPROACH**

- EPA certification cycle lifetime
- Required cycle life

**APPROACH**

- FY15
- FY16-19
The project approach has evolved based on growth in understanding of key needs and gaps, localized refinement of models, and software advancements.

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<td>Combustion modeling</td>
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<td>CFD model, fixed-temperature boundary conditions; PCP target</td>
<td>Tuning &amp; parametric studies, F-T BCs</td>
<td><strong>CHT</strong> to calculate temperature</td>
<td>Refinement and testing of CHT, with PCP target</td>
<td>Low-order model</td>
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<td>Thermo-physical properties at elevated</td>
<td>Short-term &amp; Isothermal, constant-load creep</td>
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<td><strong>Strain</strong>-based fatigue model</td>
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Objectives and Approach

Objectives

• Identify strength and fatigue performance of current HD engine materials operating at increased power densities (with higher temperatures and pressures).
• Develop methodology for defining materials properties required for lifetime of commercial HD engine operation at future extreme operating conditions.

Approach

• Use combustion Computational Fluid Dynamics (CFD) modeling to estimate temperatures and heat fluxes at current and future specific-output operating points.
• Experimentally measure relevant mechanical properties of Compacted Graphite Iron (CGI-450).
• Use Finite Element Modeling to evaluate effects of pressure and thermal environment on HD engine cylinder components of interest: head, valves, liner, piston.
  • Focus on predicted requirements for fatigue and creep on alternative (CGI-450 – HD cylinder heads) and future engine materials.
Modeling focuses on a late-model production engine

2013 15-L 6-cylinder engine; focus on single interior cylinder, up to centerlines of neighboring cylinders; based on CAD data from OEM

**Low-order combustion modeling**
- Low-dimensional treatment – less accurate, but fast → accelerates progress
- Used to complement / inform CFD simulations
  - Help define boundary conditions
  - Verify/scope trends – effort in FY18
- **GT-Power** – industry-standard simulation suite

**High-order modeling**
- More accurate, but much more computationally intensive & slow
- Industry-standard packages such as **CONVERGE** (CFD) for combustion, **ANSYS** (FEA) for structural analysis
- FE model refined from OEM-supplied FE model to focus on areas of concern

Design data from OEM and measurements; materials properties from ORNL (CGI-450 cast iron)

Both models use **solved**, rather than imposed, wall temperatures
FE was model refined to focus on stressed areas in head

Refinement gives:

► Better accuracy
► Regular temperature vs depth gradients
Summary of activities

- **Materials:** Experimentally measure relevant properties for Compacted Graphite Iron (CGI-450) at higher temperature range (up to 650–800 °C)
  - OEM-relevant and supplied material
  - Expanded temperature ranges over publicly available data (limited to ~300 °C)
  - Little creep/fatigue data publicly available at high engine temperatures

- **Progress:**
  - Tensile strength, thermal diffusivity, coefficient of thermal expansion, critical temperatures, specific heats
  - Short-term creep
  - Isothermal, constant-load creep
  - High-temperature fatigue

- **Combustion:** Evaluated model for three PCP ranges based on **specific-power increase trajectories:** 190 (baseline), 225–250 bar & >250 bar, using two materials (Gray Cast Iron & CGI-450).

- **Key findings:**
  - Temperatures ~20–30 °C higher for CGI than Gray Cast Iron (thermal conductivity)
  - Temperatures ~25–50 °C higher at mid-range specific-power increase (~225–240 bar)
FE model load was applied in a series of steps

FEA model examined four load scenarios, allowing decomposition of load effects on resulting stresses and strains.

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<th>Step</th>
<th>Load</th>
<th>Scenario</th>
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<tr>
<td>1</td>
<td>Preload</td>
<td>Cold engine, engine off (head bolts cause preload)</td>
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<tr>
<td>2</td>
<td>Preload + Pressure</td>
<td>Cold engine, combustion pressure</td>
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<tr>
<td>3</td>
<td>Preload + Temperature</td>
<td>Hot engine, no combustion pressure</td>
</tr>
<tr>
<td>4</td>
<td>Preload + Pressure + Temperature</td>
<td>Hot engine, full combustion effects</td>
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FEA predicts temperature has a greater impact on stresses than pressure.

Stresses are in [psi]

Conditions: CGI, 190 bar operation, elastic-only model

EV: Exhaust valve
IV: Intake Valve
FI: Fuel Injector
Baseline FEA scenarios suggest stresses greater than yield

Conditions: **CGI**, 190 bar operation, elastic-only model

Plasticity must be accounted for in model (achieved this FY using ORNL experimental data).
FEA predicts lower stresses in the presence of plasticity

Stresses, elastic-only model

Note: color maps on different scales

Stresses, model with plasticity

Stresses are in [psi]

Conditions: CGI, 190 bar operation

EV: Exhaust valve
IV: Intake Valve
FI: Fuel Injector

Plasticity must be accounted for in model when evaluating engine-component lifespan.
Temperature increases with combustion intensity

- High-flux scenario 25% more heat flux from combustion (~225 bar PCP range)
- Cooling heat-transfer coefficient adjusted to explore effects on materials temperatures (no material changes)

**Key findings:**
- Temperatures greatly increase with heat flux
- Cooling alone cannot counteract heat-flux effects
- Similar trends seen with Gray Cast Iron, but ~25 °C cooler
Engines will be distressed with higher specific output

- Extreme temperatures and stresses extend 1–2 mm (10–15%) into the fire deck
- Plasticity is observed under these temperatures and stresses
- Creep will be an additional concern under these conditions and is not accounted for in these models

Temperatures in exhaust valve bridge

Baseline (190 bar PCP) High flux (~225 bar PCP)

Strain in head for CGI for baseline (L) and high-flux (R) conditions

Conditions: CGI, model with plasticity

EV: Exhaust valve
IV: Intake Valve
FI: Fuel Injector
Summary of findings

Combustion

• For this engine design and operating strategy, ~25% greater combustion heat flux results in 225–240 bar operation
• Temperatures rise by 25–50 °C at higher specific-power operation
• CGI experiences ~20–30 °C higher temperatures just from thermal conductivity differences compared with engine-grade gray cast iron

Materials

• Temperature has a significant effect on stresses developed in the head
• Stresses in head reach plastic regime, so models must account for plasticity
• Higher temperatures and stresses at higher engine specific output suggest that creep is expected to be a greater concern
Future work may extend methods to other domains

• Complete heavy duty, transfer methodology

• Focus on light-duty engines
  • Lightweight materials constraints have implications
  • Different architectures
  • Different combustion strategies
  • Lower service-life environment with lower cost margins
Responses to Prior-Year Comments

Comment: Combined treatment of fatigue and creep should be developed, focusing on residual stresses left by the heating–cooling cycles, which can lead to crack initiation.

Response: We are now completing the analysis at the highest combustion heat loading and intend to complete the overall cycle analysis by accounting for low-load and transient conditions.

Comment: Collaborations and interactions should be more explicitly stated.

Response: We mention the degree of collaborations but not specific names or roles to protect sensitivities of some collaborators.
Collaborations

Data exchange
– An OEM provided operating data for validation of HD model

Model exchange
– An OEM provided initial FE model
– ORNL shared FEA results with an OEM

Materials
– An OEM provided materials for properties measurements at ORNL
– ORNL shared materials properties measurements with an OEM
Summary

Relevance
• Directly addressing materials barriers to enable advanced engine and powertrain systems for propulsion applications

Approach
• Apply computational methods linking experiments and numerical simulations to accelerate materials selection and development
• Extend capabilities to address problems using novel approaches

Accomplishments
• Progressed on state-of-the-art co-simulation of combustion and materials thermal properties
• Decomposed effects of pressure and temperature on stresses and strains in two materials
• Evaluated roles of material and design on temperatures, stresses, and strain
• Continued measurement of materials properties of CGI-450 at engine-relevant temperatures

Collaborations
• Collaborations with industry partners are producing shared materials and ideas that are relevant to commercial application in next-generation powertrains

Future work
• Specify workflow for determining future HD engine operation to meet lifespan needs
• Transition methodology to projects evaluating LD engines

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Any proposed future work is subject to change based on funding levels