Oak Ridge National Laboratory

Applied Computational Methods for New Propulsion Materials

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Project Overview

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

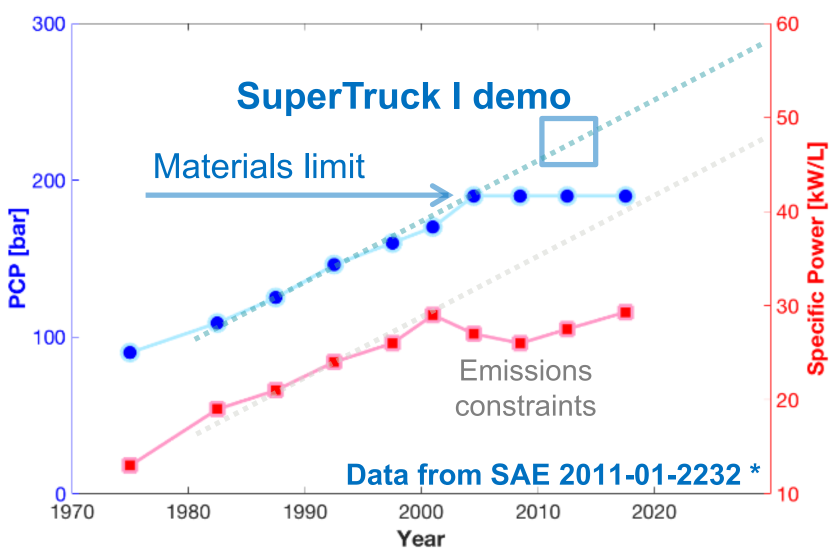
- FY2017 – $235 K
- FY2018 – $230 K
- FY2019 – $210 K

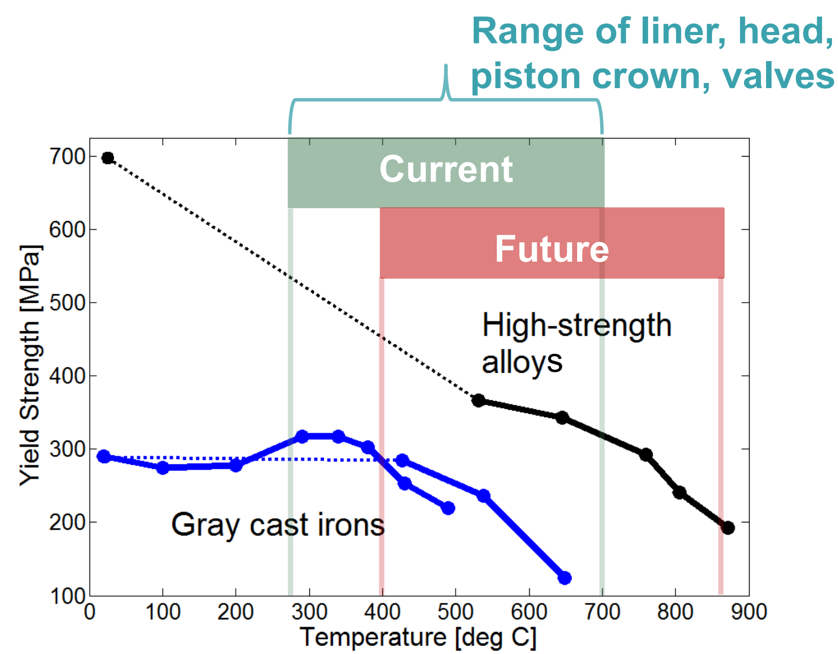
Partners

- **Convergent Science, Inc.**
- **Two engine OEMs**

Power-density trends in HD engines present challenges for materials with higher temperatures and pressures

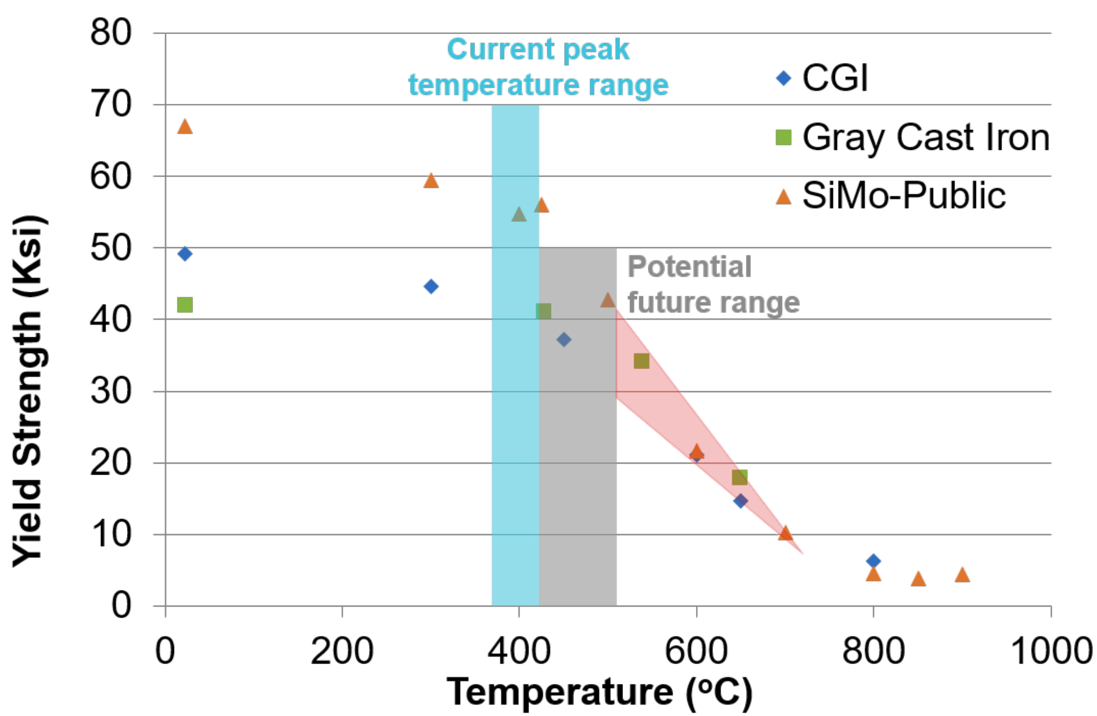
- **Trend**: Roadmap for heavy-duty (HD) engine operation projects increasing specific output, with **higher peak cylinder pressures** (PCP) and **temperatures** into the foreseeable future
  - SuperTruck I programs showed >50% BTE with ≈225 bar PCP, for short timespans
- **Challenge**: **Materials properties degrade with temperature**
  - ❖ Concerns: Strength, creep, fatigue, oxidation/corrosion, cost



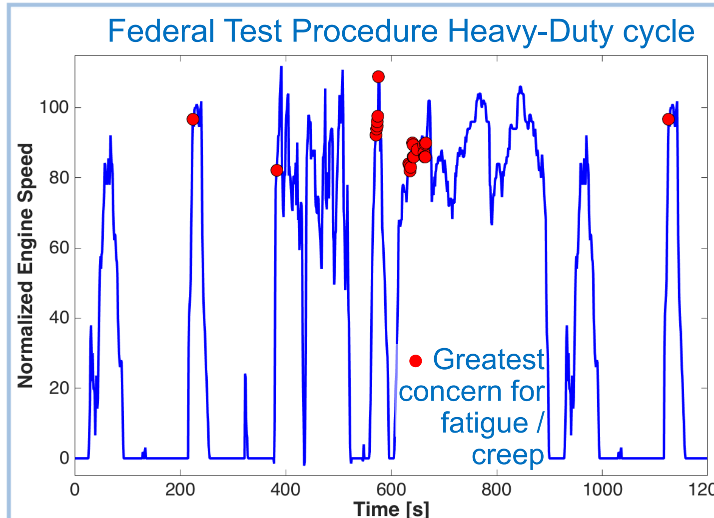


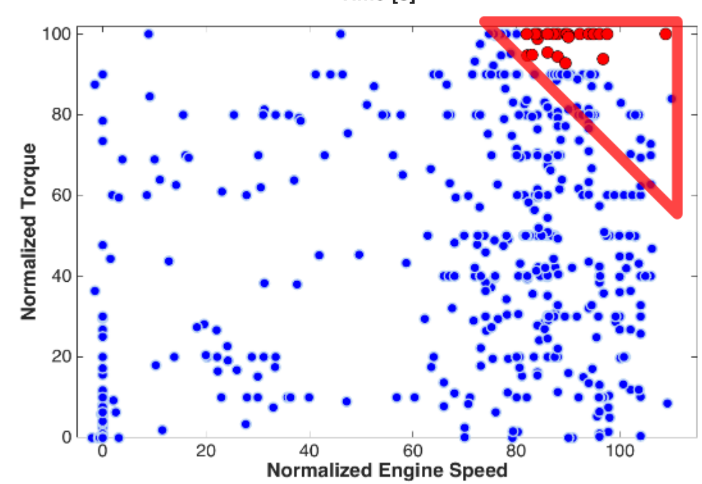
* M. Megel *et al*. (2011). SAE 2011-01-2232; *SAE Int. J. Engines* **4**(3).

Many cast irons have similar tensile properties at elevated temperatures, but creep and fatigue life are also important



Many cast irons have similar properties, such as yield strength, in anticipated future operating conditions.





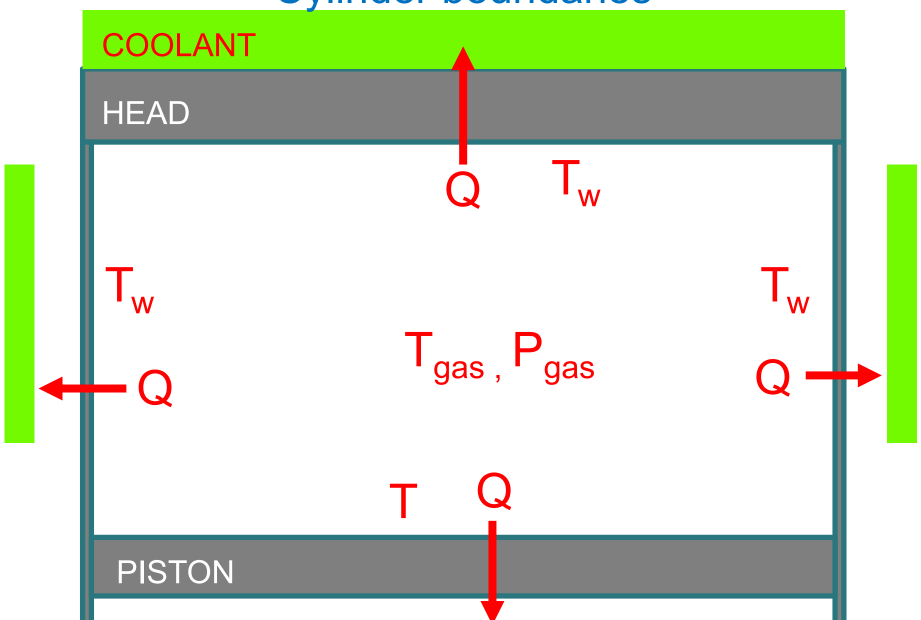
Only a small portion of an engine's duty cycle has the greatest impact on materials lifespan.

Additional materials properties, including fatigue life, determine suitability for more intensive engine applications.

Gas-materials interface is important in engine modeling, analysis, and operation

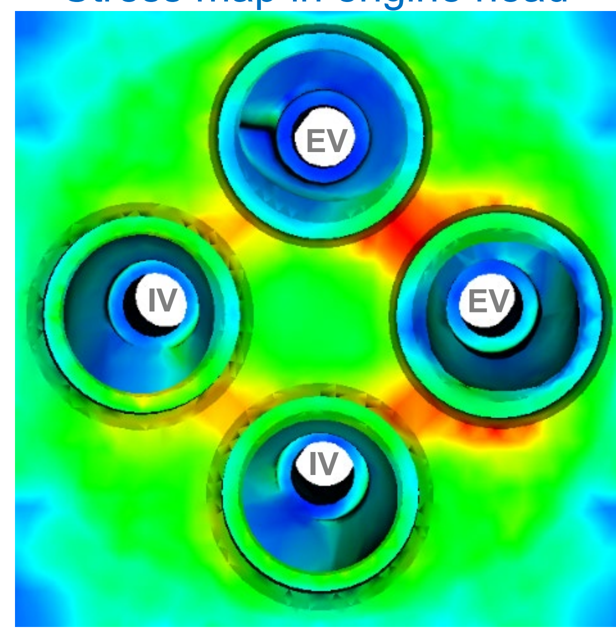
- Cylinder walls contain combustion gases, provide heat-transfer interface
  - Extreme environment has impact on materials (e.g., corrosion, stresses)
- Spatially varying heat flux is important in evaluating materials stresses
- Traditional combustion modeling uses specified boundary conditions
- Advances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

Cylinder boundaries



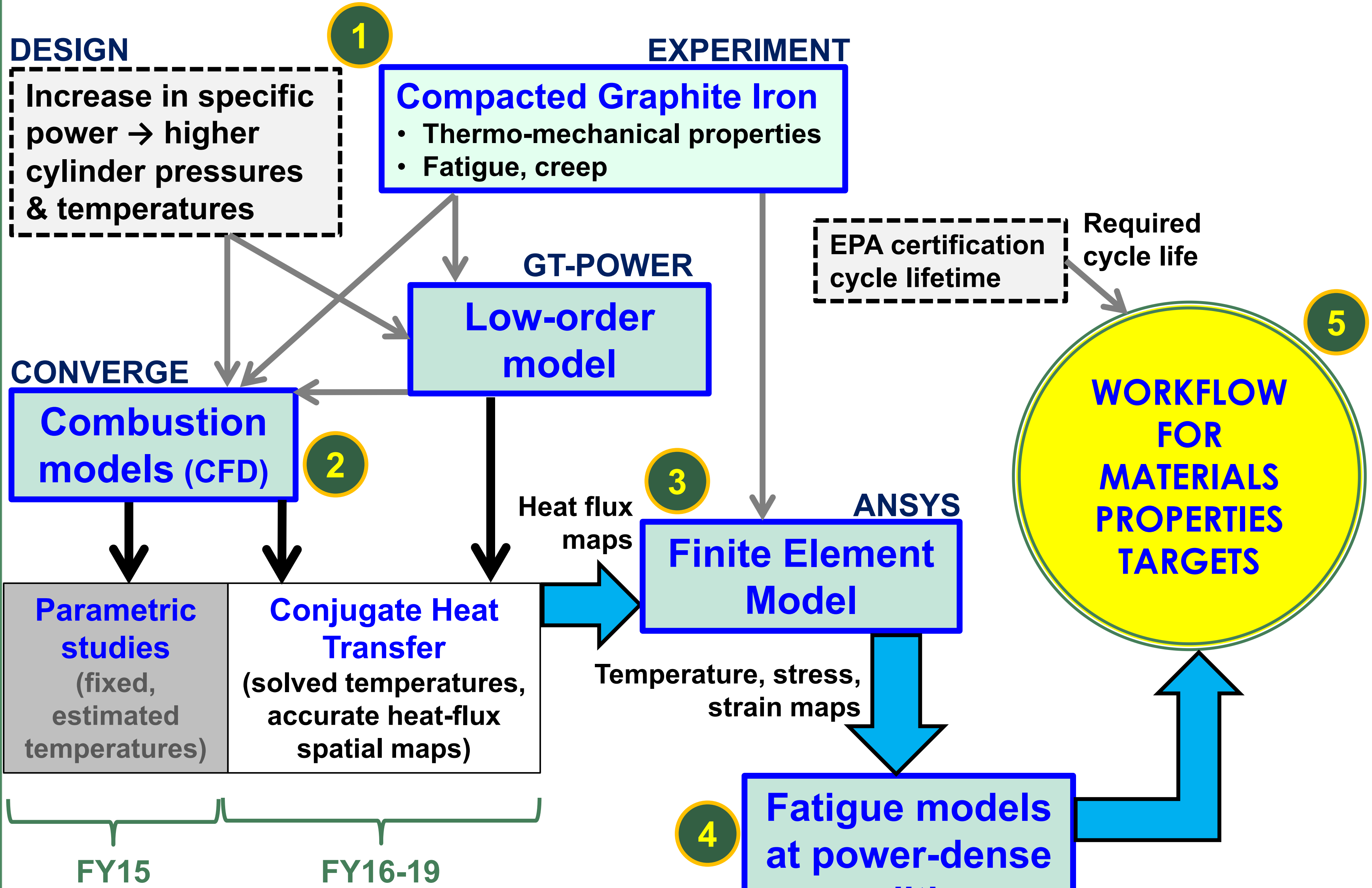
Q : heat transfer
T : temperature
P : pressure

Stress map in engine head



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

This project integrates experiment and modeling



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

FY2014	FY2015	FY2016	FY2017	FY2018	FY2019
Combustion modeling					
CFD model, **fixed-temperature** boundary conditions; **PCP target**	Tuning & parametric studies, F-T BCs	**CHT** to calculate temperature	Refinement and testing of CHT, with PCP target	Low-order model Switch to **power-density target**	Low-order model with 3D CHT CFD finalized
Materials characterization					
	Materials from OEM	Thermo-physical properties at elevated	Short-term & Isothermal, constant-load creep	Isothermal, constant-load creep High-T fatigue	
Structural modeling					
Baseline FEA, partial refinement				Refinement of FE model for targeted results	Evaluating materials and operating effects **Strain**-based fatigue model

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

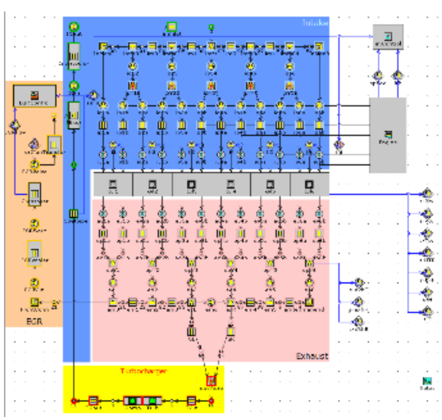
2013 15-L 6-cylinder engine; focus on single interior cylinder, up to centerlines of neighboring cylinders; based on CAD data from OEM

Low-order combustion modeling

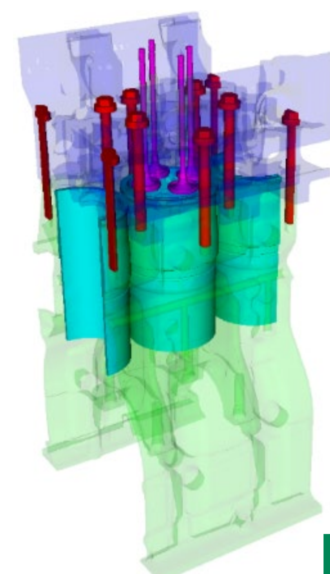
- Low-dimensional treatment – less accurate, but fast → accelerates progress
- Used to complement / inform CFD simulations
  - Help define boundary conditions
  - Verify/scope trends – effort in FY18
- **GT-Power** – industry-standard simulation suite

High-order modeling

- More accurate, but much more computationally intensive & slow
- Industry-standard packages such **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)

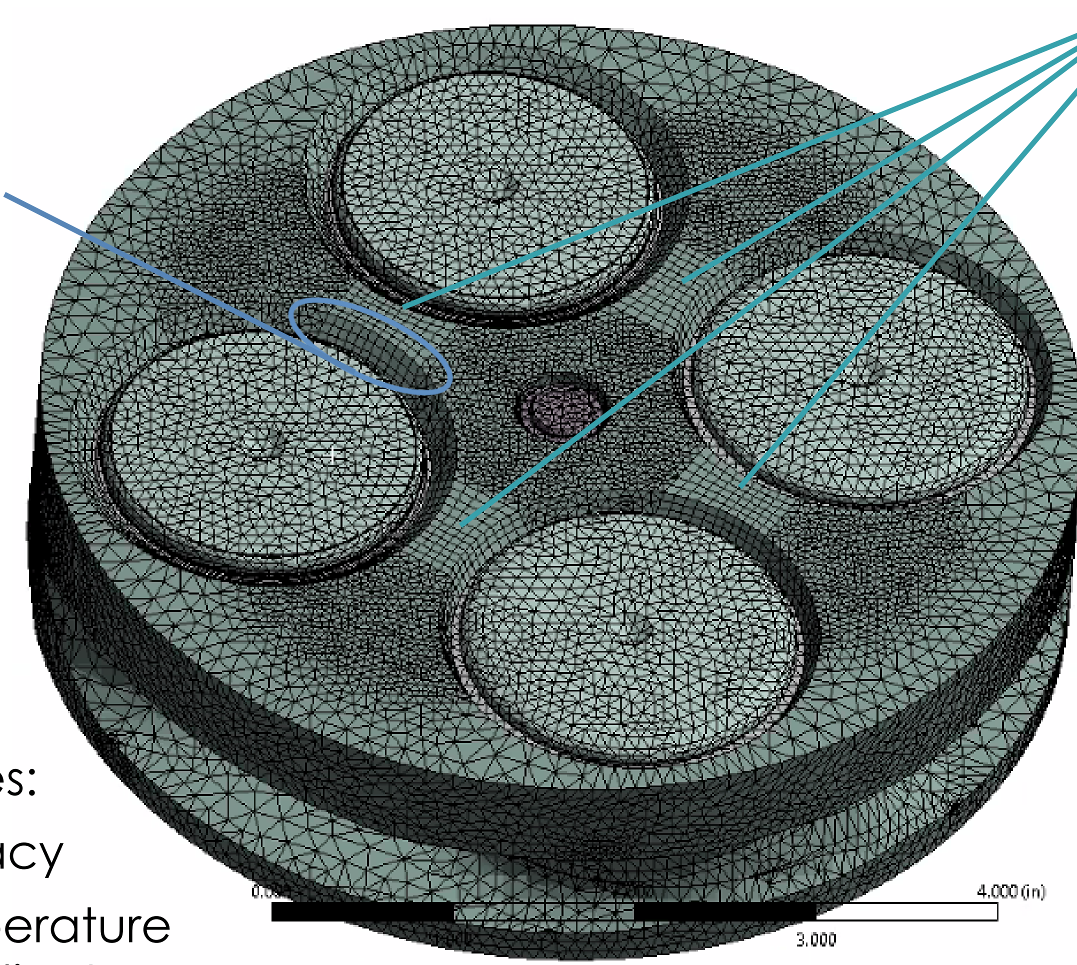


Both models use <u>solved</u>, rather than imposed, wall temperatures

FE was model refined to focus on stressed areas in head

Regular elements placed in bridges between valves

Layers of regular hex elements extended into head close to cooling channels



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)**

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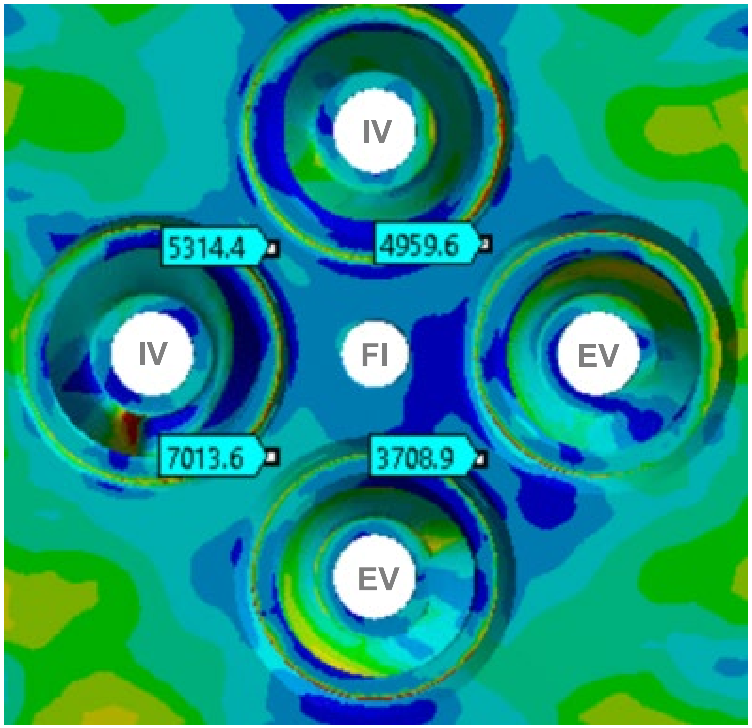
TECHNICAL ACCOMPLISHMENT

FE model load was applied in a series of steps

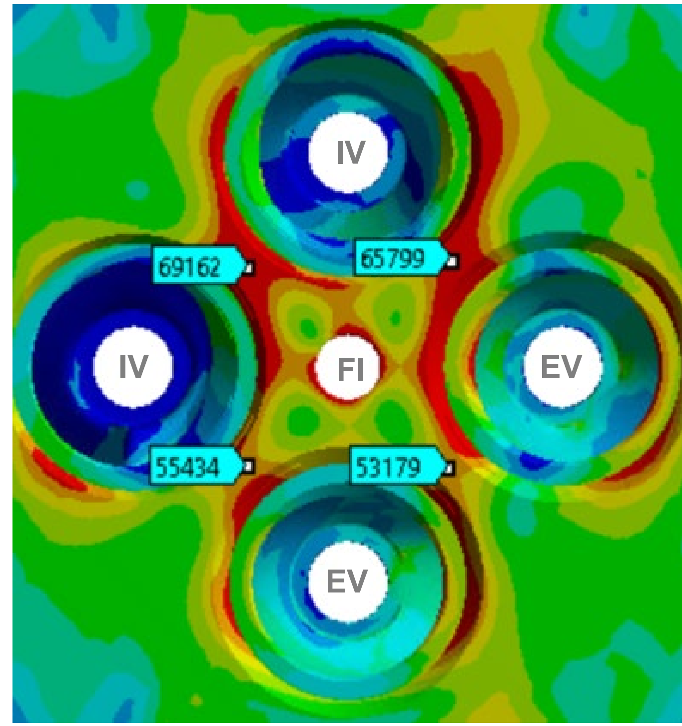
FEA model examined four load scenarios, allowing decomposition of load effects on resulting stresses and strains.

Step	Load	Scenario
1	Preload	Cold engine, engine off (head bolts cause preload)
2	Preload + Pressure	Cold engine, combustion pressure
3	Preload + Temperature	Hot engine, no combustion pressure
4	Preload + Pressure + Temperature	Hot engine, full combustion effects

FEA predicts temperature has a greater impact on stresses than pressure



Preload + Cylinder Pressure Load



Preload + Combustion Temperature Rise

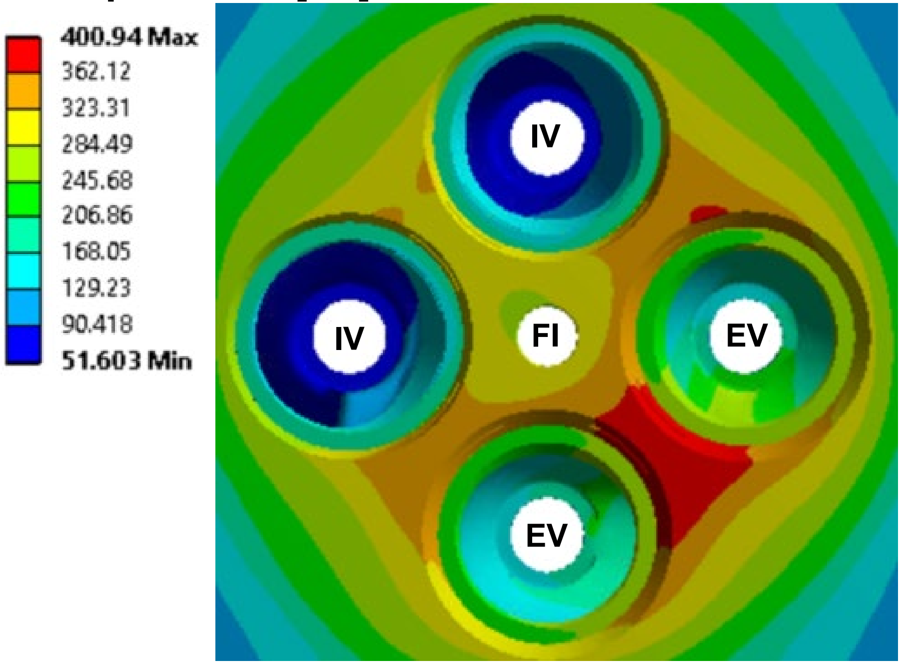
Stresses are in [psi]

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

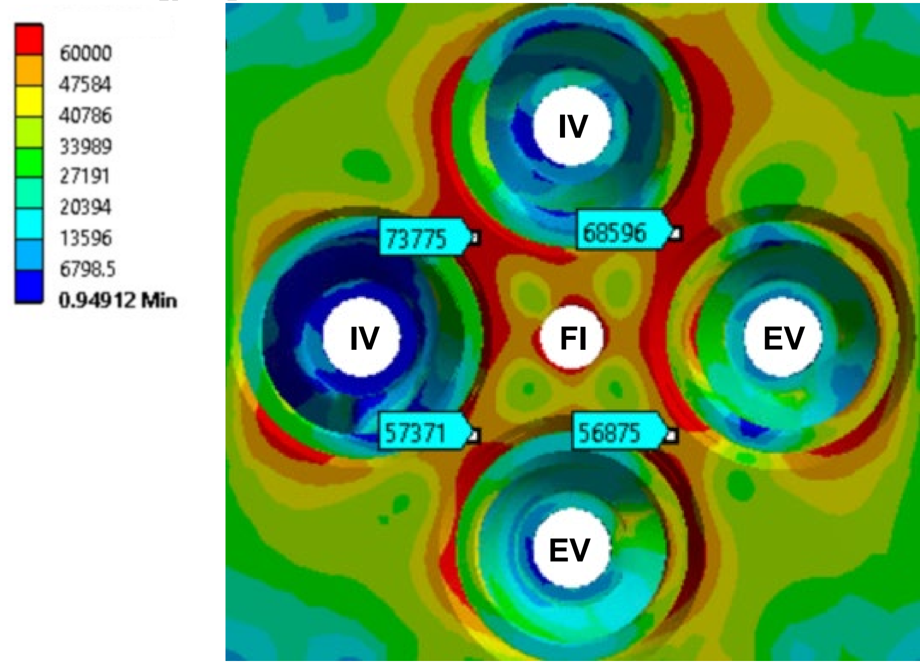
EV: Exhaust valve
IV: Intake Valve
FI: Fuel Injector

Baseline FEA scenarios suggest stresses greater than yield

Temperature [°C]



Stress [psi]



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

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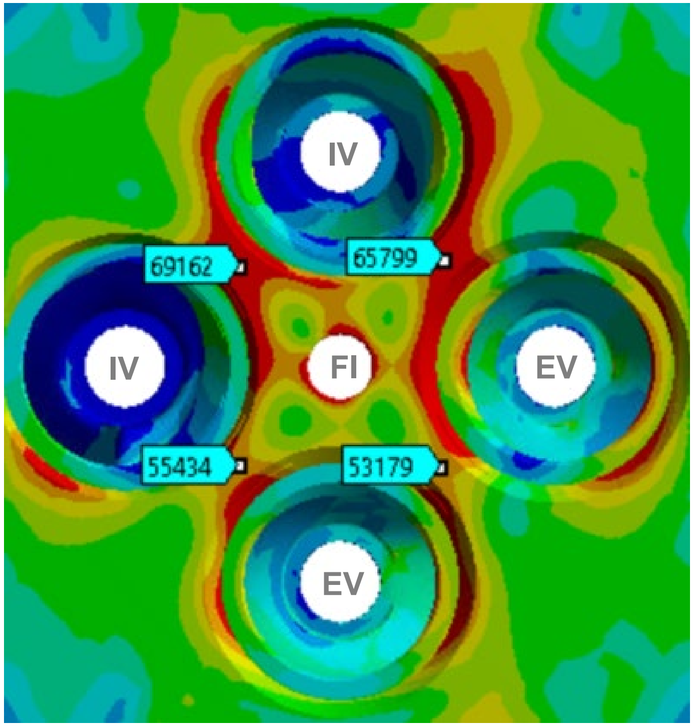
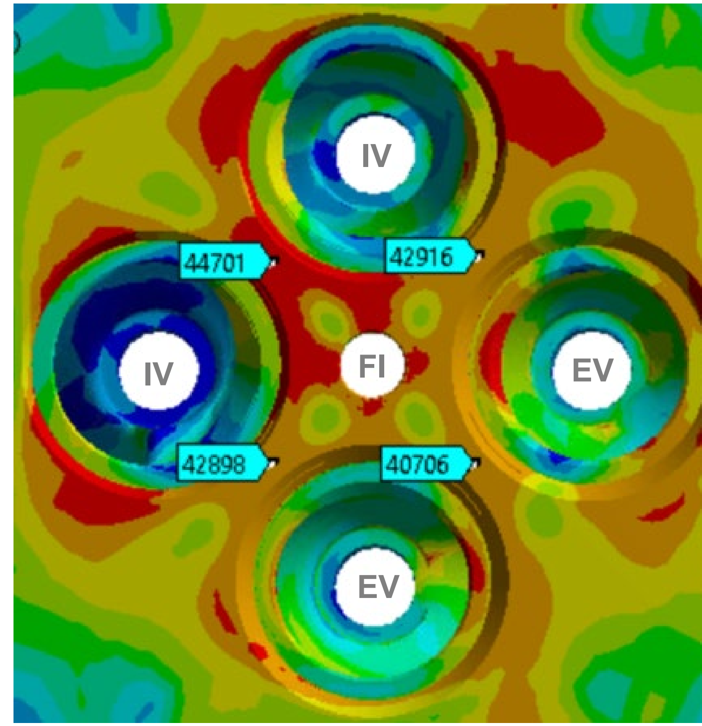
Plasticity must be accounted for in model (achieved this FY using ORNL experimental data).

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.

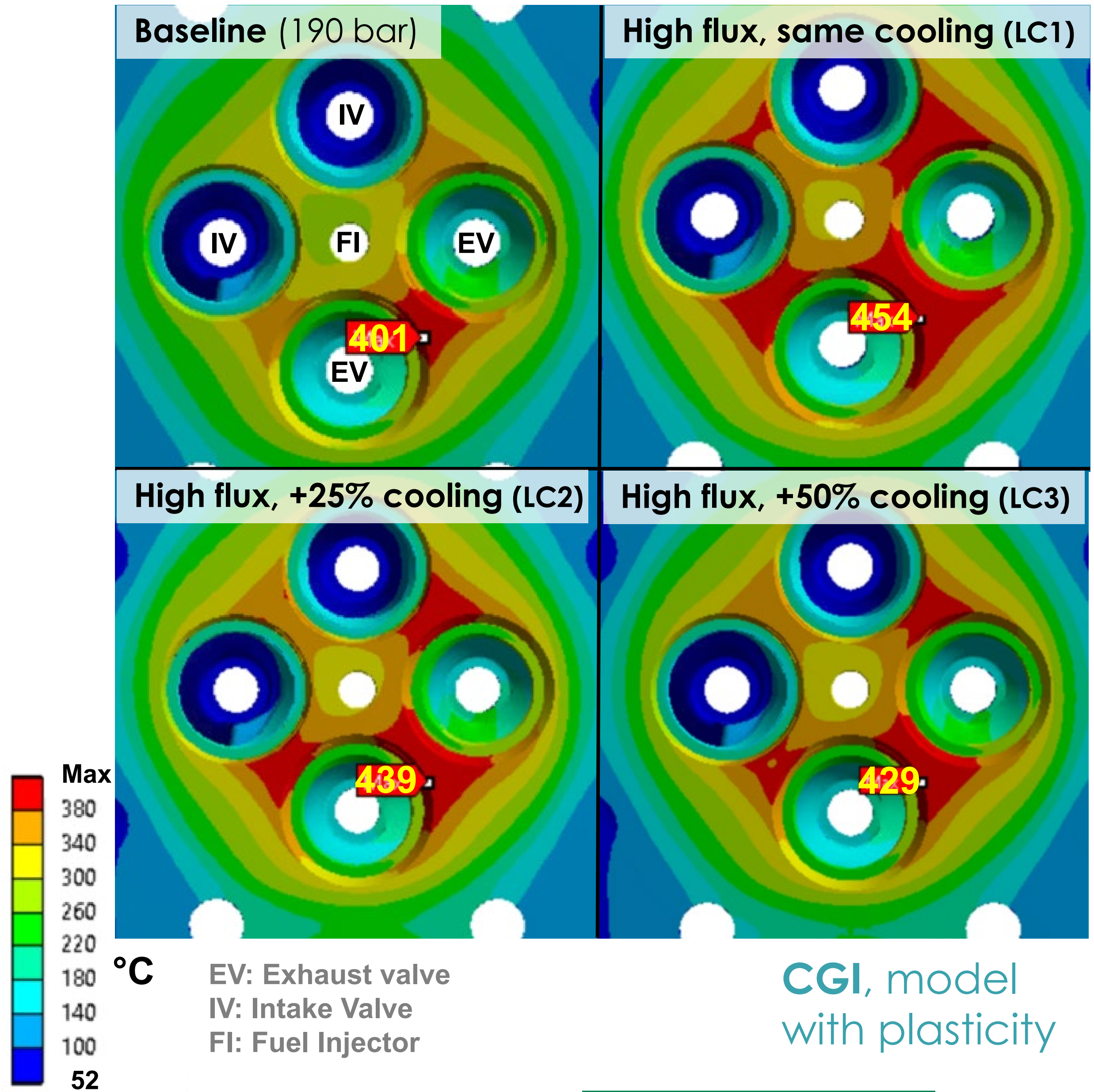
TECHNICAL ACCOMPLISHMENT

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

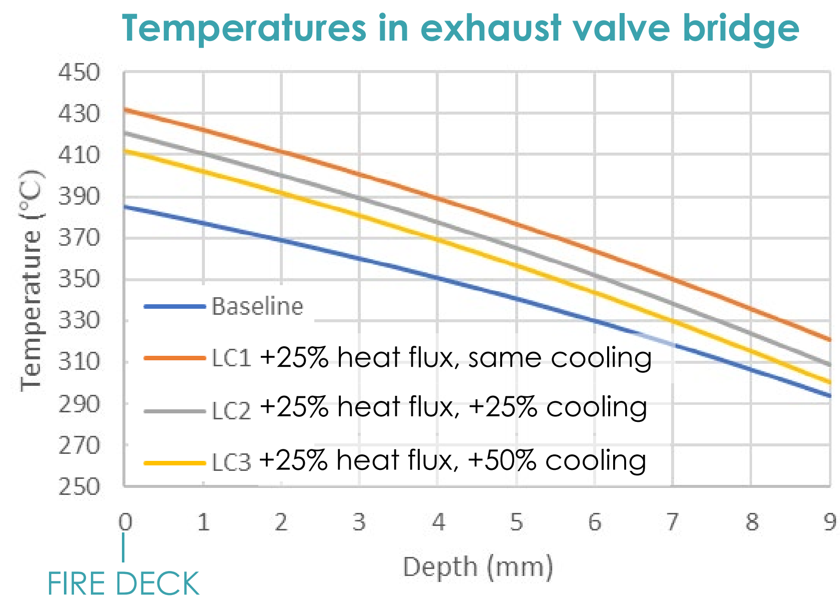


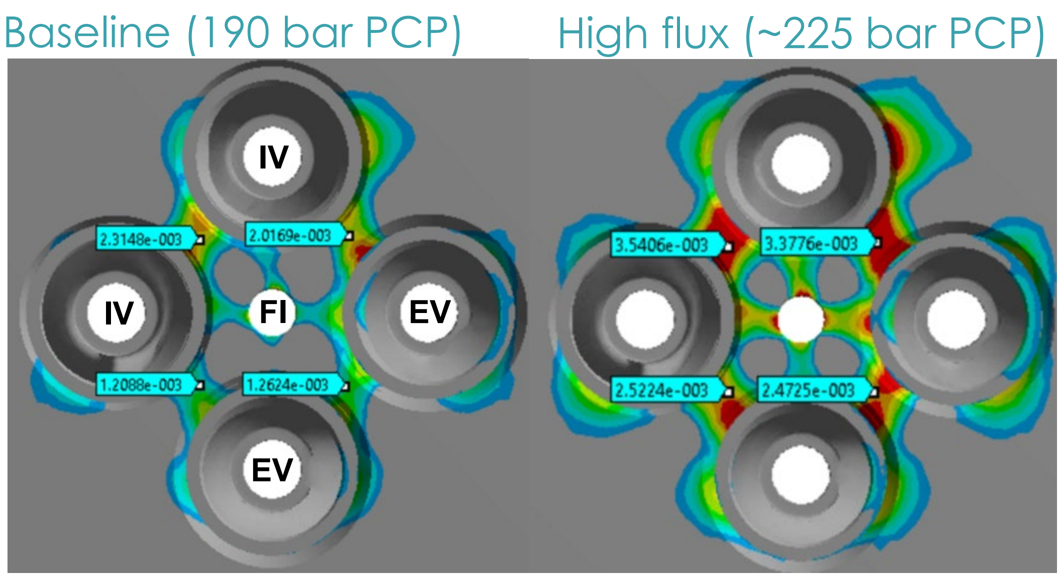
EV: Exhaust valve
IV: Intake Valve
FI: Fuel Injector

CGI, model with plasticity

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**





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

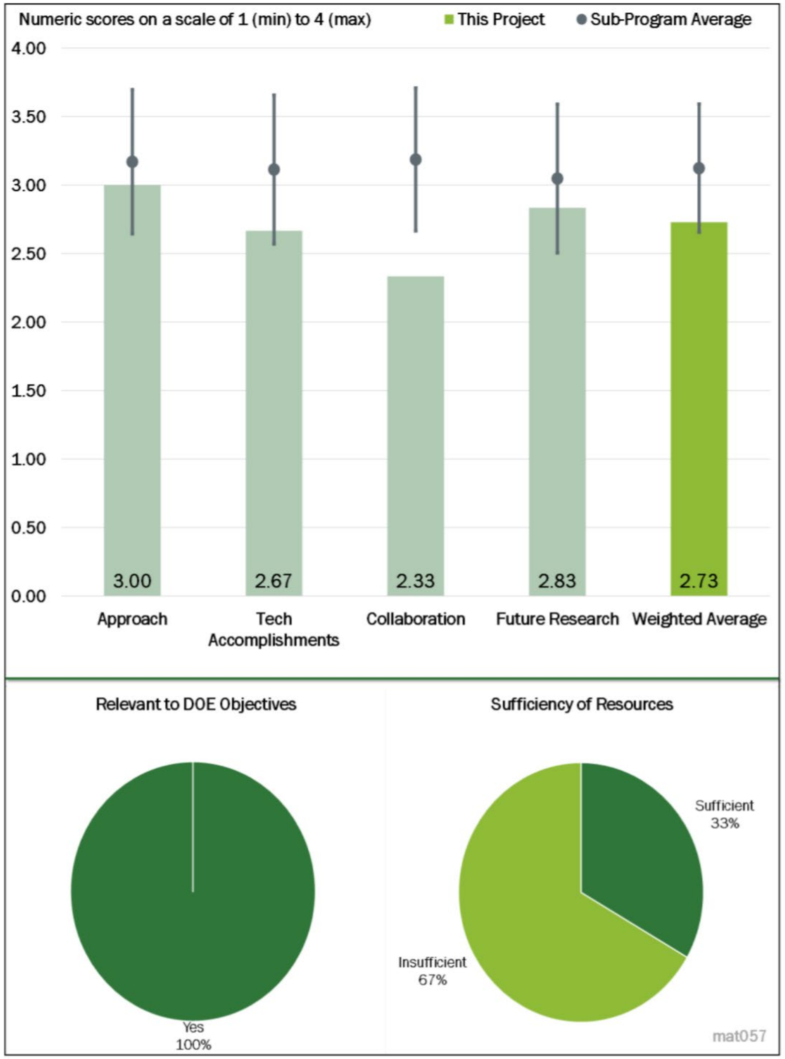
Materials

- 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



<u>Comment</u>: 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.

<u>Response</u>: 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.

<u>Comment</u>: Collaborations and interactions should be more explicitly stated.

<u>Response</u>: 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

Contact:
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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

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