Applied Computational Methods for
New Propulsion Materials

Future engine requirements

Charles E.A. Finney

Email: finneyc@ornl.gov
Phone: 865-946-1243

Govindarajan Muralidharan
Zachary G. Mills
J. Allen Haynes

Oak Ridge National Laboratory

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Project Overview

Timeline

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

Barriers

- **Directly targets barriers identified in the 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

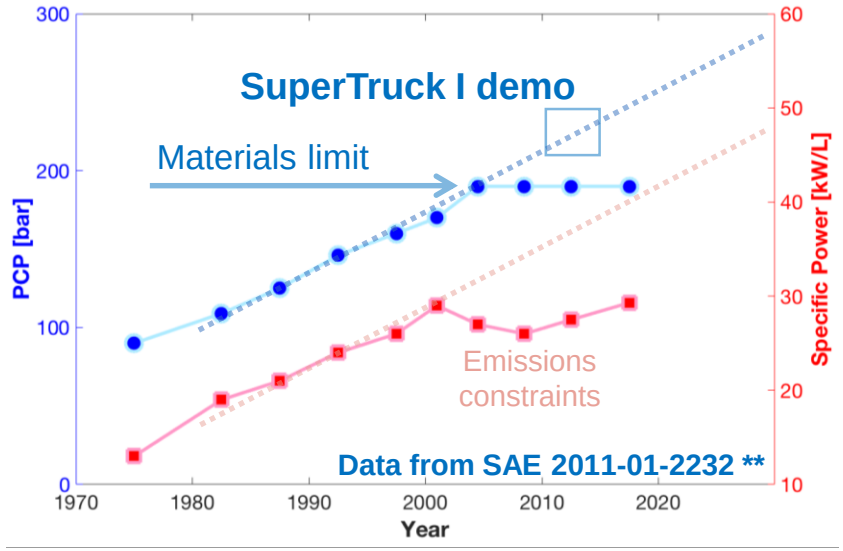
- FY2016 – $140 K
- FY2017 – $235 K
- FY2018 – $230 K

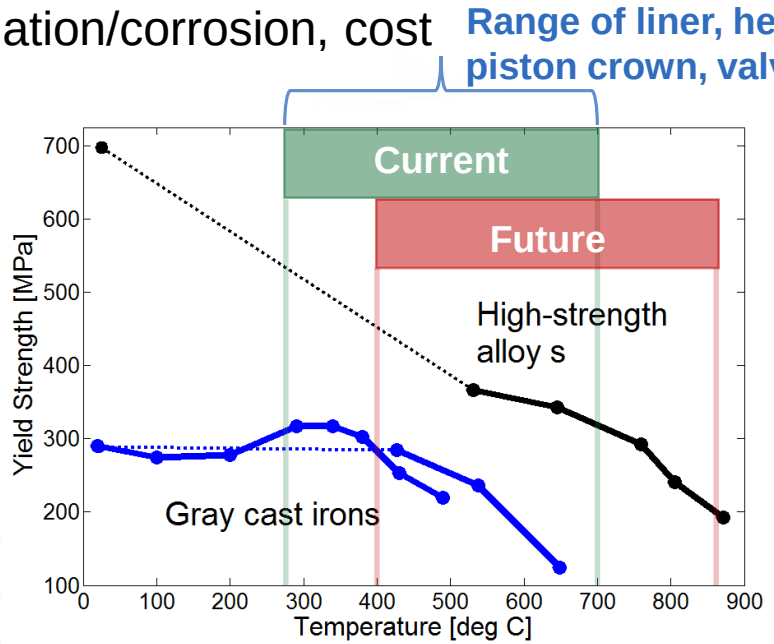
Partners

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

Enabling higher operating pressures is part of trend to increase power density and efficiency

- Multi-Year Program Plan* Task: Evaluate and characterize emerging materials for application in advanced high-efficiency heavy truck engines
- Roadmap for heavy-duty (HD) engine operation projects increasing specific power, 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
  - Materials properties degrade with temperature
    - ❖ Concerns: Strength, creep, fatigue, oxidation/corrosion, cost





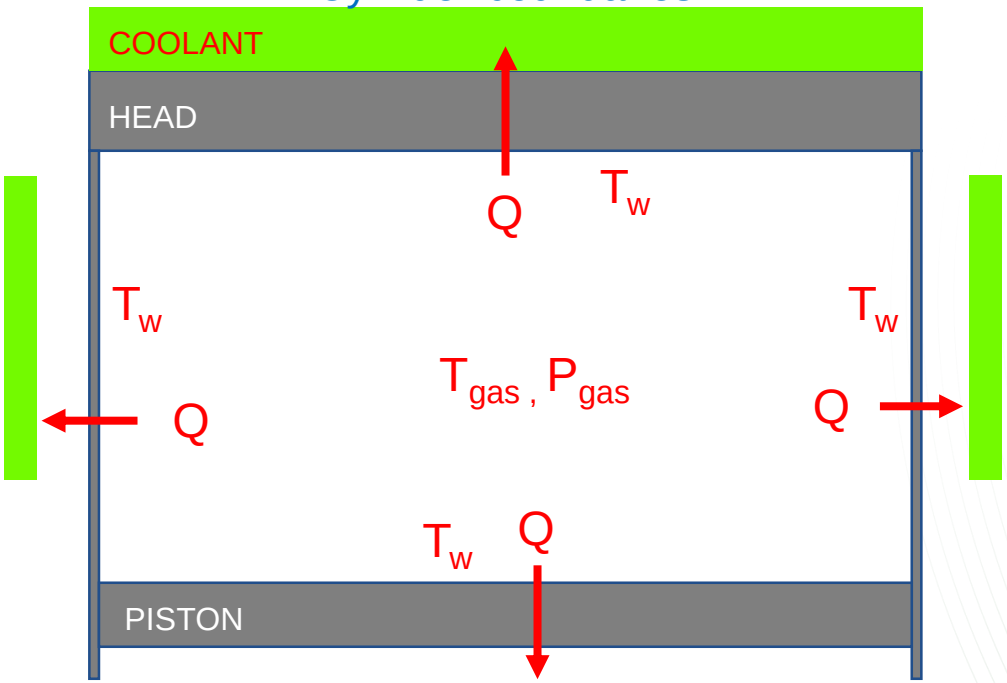
* Vehicle Technologies Program Multi-Year Program Plan (2011-2015).
** M. Megel *et al*. SAE 2011-01-2232; *SAE Int. J. Engines* **4**(3).

RELEVANCE

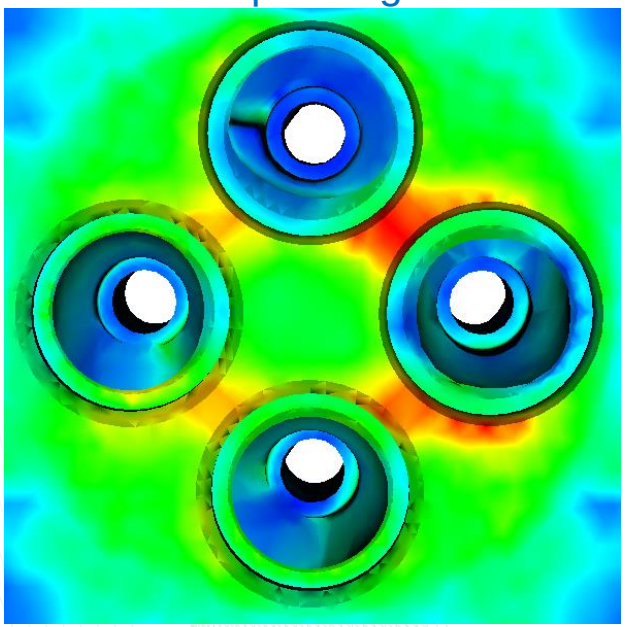
Gas-materials interface is important in engine modeling, analysis, and operation

- Cylinder surfaces contain combustion gases and provide heat-transfer interface
  - Extreme environment has impact on materials (e.g., corrosion, oxidation, stresses)
- Traditional modeling uses specified boundary conditions; advances in simulation now support temperature and more accurate heat-flux co-solution of gases and structure solids
- Spatially varying heat flux is important in evaluating materials stresses

Cylinder boundaries



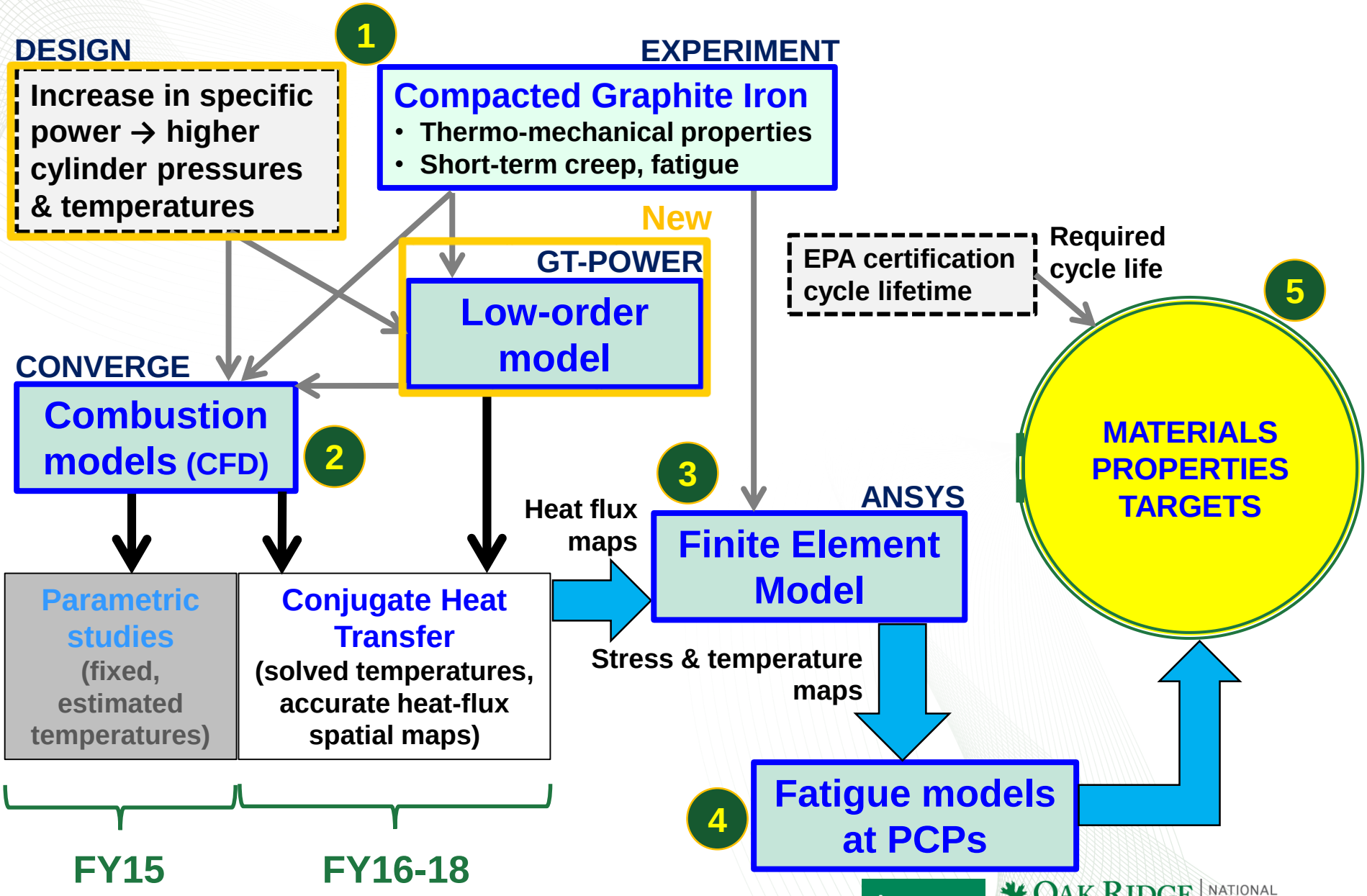
Stress map in engine head



NB: Injector removed (lower resultant stresses)

Q : heat transfer | T : temperature | P : pressure

This project integrates experiment and modeling



Objectives and Approach

Objectives

- Identify strength and fatigue performance of current HD engine materials operating at elevated peak cylinder pressures (PCP) and temperatures.
- Define materials properties required for lifetime of commercial HD engine operation at future extreme operating conditions.

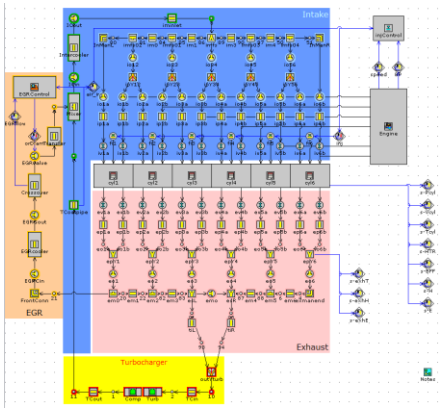
Approach

- Use combustion Computational Fluid Dynamics (CFD) modeling to estimate temperatures and heat fluxes at current and future PCP operating points.
- 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 of fatigue properties analysis and factors of safety on alternative (Compacted Graphite Iron – HD cylinder heads) and future engine materials

Modeling Approach

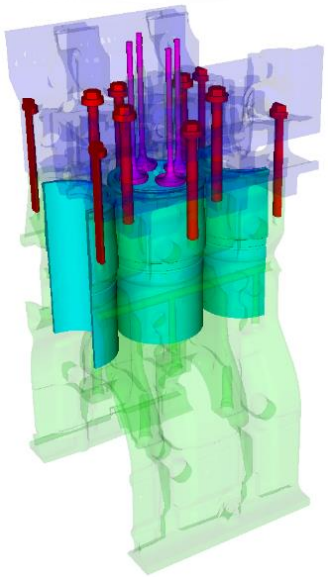
Low-order modeling

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



High-order modeling

- Engine: 2013 15-L 6-cylinder engine; focus on single interior cylinder, up to centerlines of neighboring cylinders; based on CAD data from OEM
- More accurate, but slow
- Interfacing industry-standard packages such **CONVERGE** (CFD), **ANSYS** (FEM)



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

Both models use solved rather than imposed wall temperatures

Computational demands soon will necessitate HPC

Workstation scale (current)

- Stretching the limits of workstation
  - ~5–10 GB per core
  - >2 weeks continuous for single case

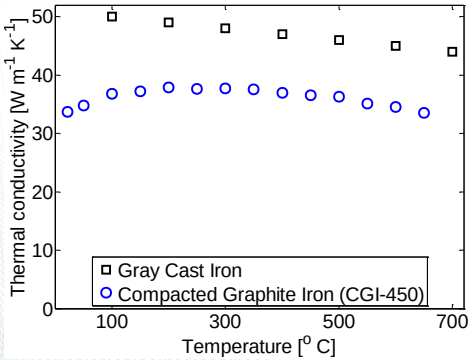
HPC potential (future)

- Simulations do not scale well to current, traditional supercomputers due to core memory requirements (1–2 GB/core), resource limitations
- Massively parallel Design of Experiments best application
- Future HPC architectures (Summit) will be better-suited

Activities and Progress – Materials characterization

- Experimentally measure relevant properties for Compacted Graphite Iron (CGI-450) at an expanded range of temperatures (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 [complete FY16]
  - Short-term creep [complete FY17]
  - Isothermal, constant load creep [in progress]
  - High-temperature fatigue [in progress]
  - Constitutive model for CGI-450 [under development]

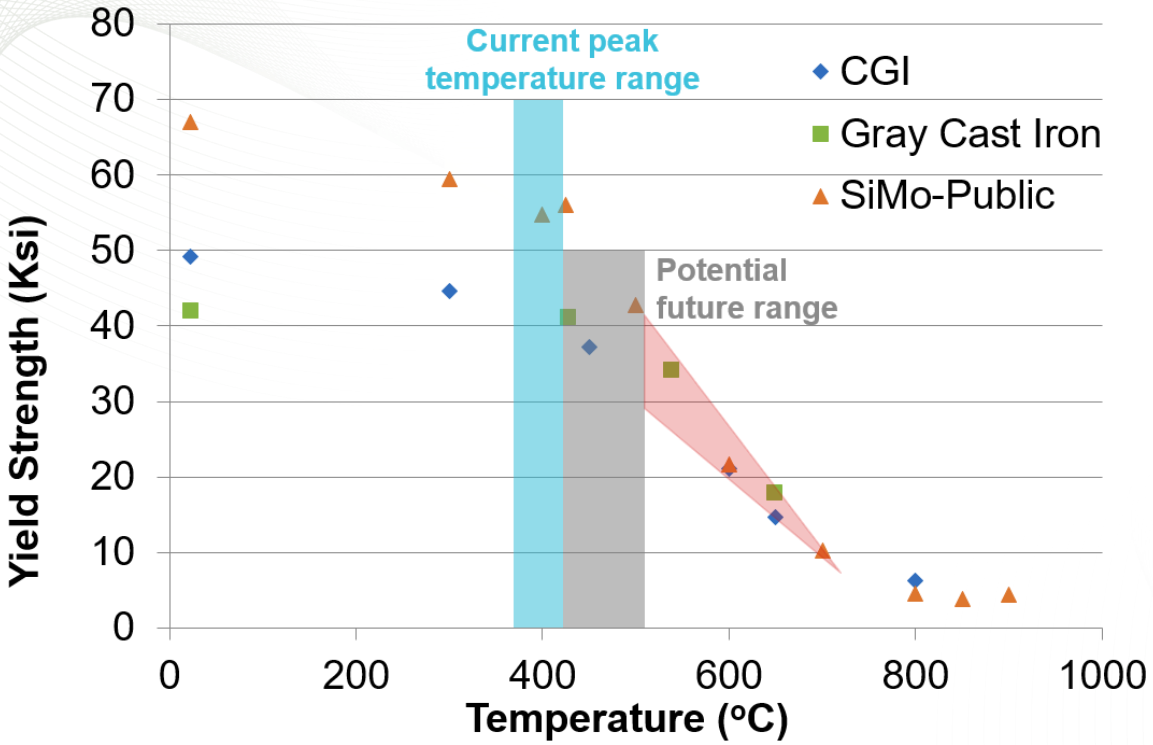
Utility:
- Assists engine-design community
- Used in this project's modeling efforts



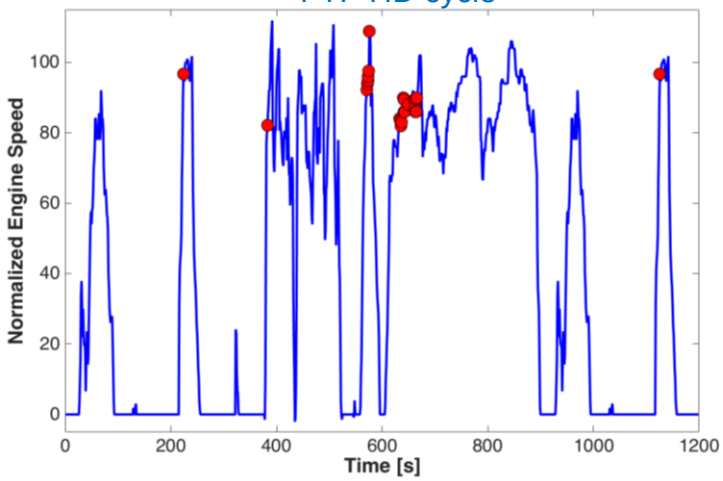
Thermal conductivity versus temperature of CGI-450 (ORNL) is lower than Gray Cast Iron (reference)

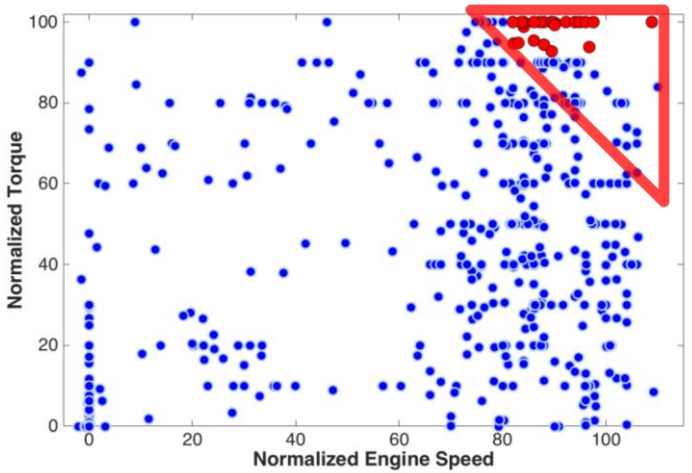
TECHNICAL ACCOMPLISHMENT

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



FTP HD cycle



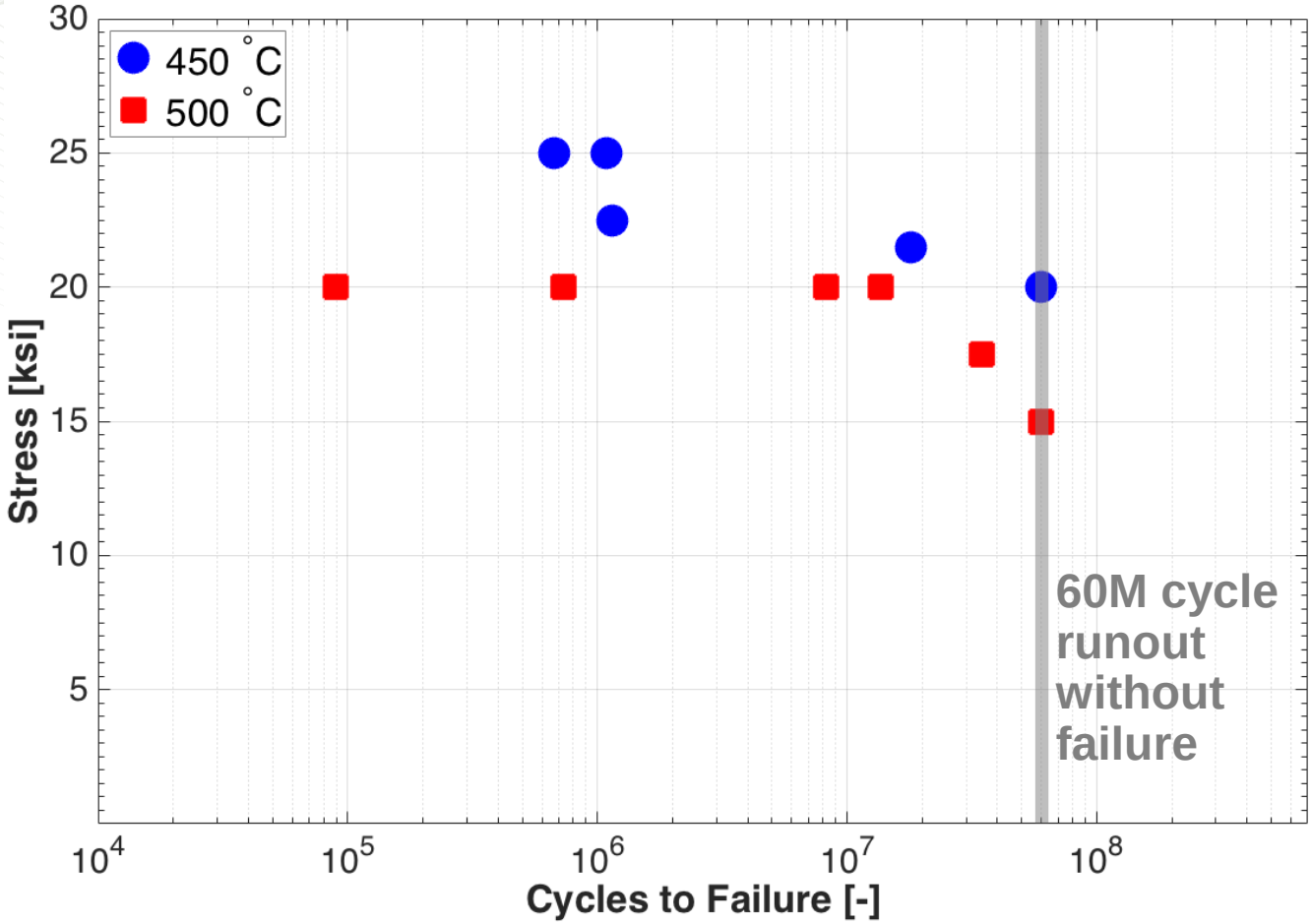


● Greatest concern for fatigue life

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

RELEVANCE/PRIOR-YEAR TECHNICAL ACCOMPLISHMENT

Fatigue life is very sensitive to stress at projected temperatures



Preliminary, ongoing ORNL CGI-450 fatigue measurements at elevated temperatures

Ongoing creep studies suggest that high creep rates at T > 400 °C correlate with degraded fatigue life.

TECHNICAL ACCOMPLISHMENT

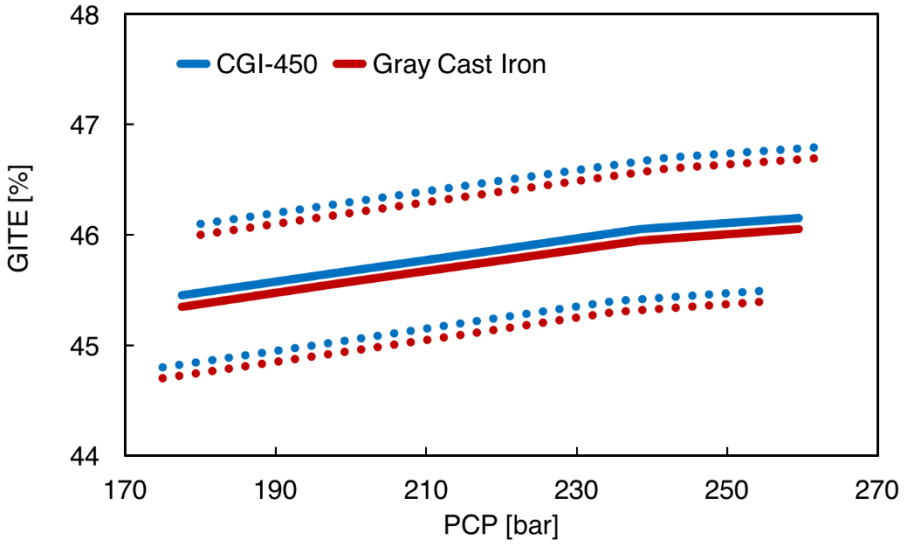
Activities and Progress – Combustion modeling

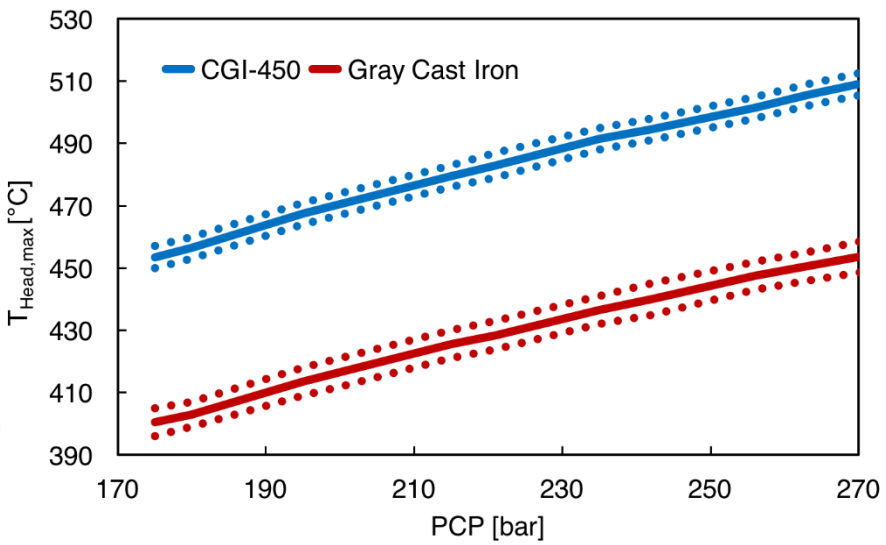
- Dual-track modeling underway:
  - Low-order: Scope problem and verify trends for CFD
  - High-order: Increase accuracy and spatial resolution of temperature-stress maps
- Conjugate heat transfer (CHT) modeling to solve combustion and materials temperatures iteratively, for accurate thermal spatial distribution
- Evaluation of model for three PCP ranges based on **specific-power increase trajectories**: **190** (current practice), **225–250** bar & >**250** bar, using two materials (Gray Cast Iron & CGI-450).

Utility:
- Define thermal environment for FEM
- Estimate indicated efficiencies to quantify benefits of high PCP

Activities and Progress – Low-order combustion modeling

- Combustion intensification can yield higher specific power and efficiency but raises materials temperatures
- Material properties (e.g., thermal diffusivity) affect combustion and heat transfer
- Target regime represents <5 % of engine lifetime duty cycle but has the limiting materials requirements





Trends with increasing specific power

GT-Power simulations

TECHNICAL ACCOMPLISHMENT

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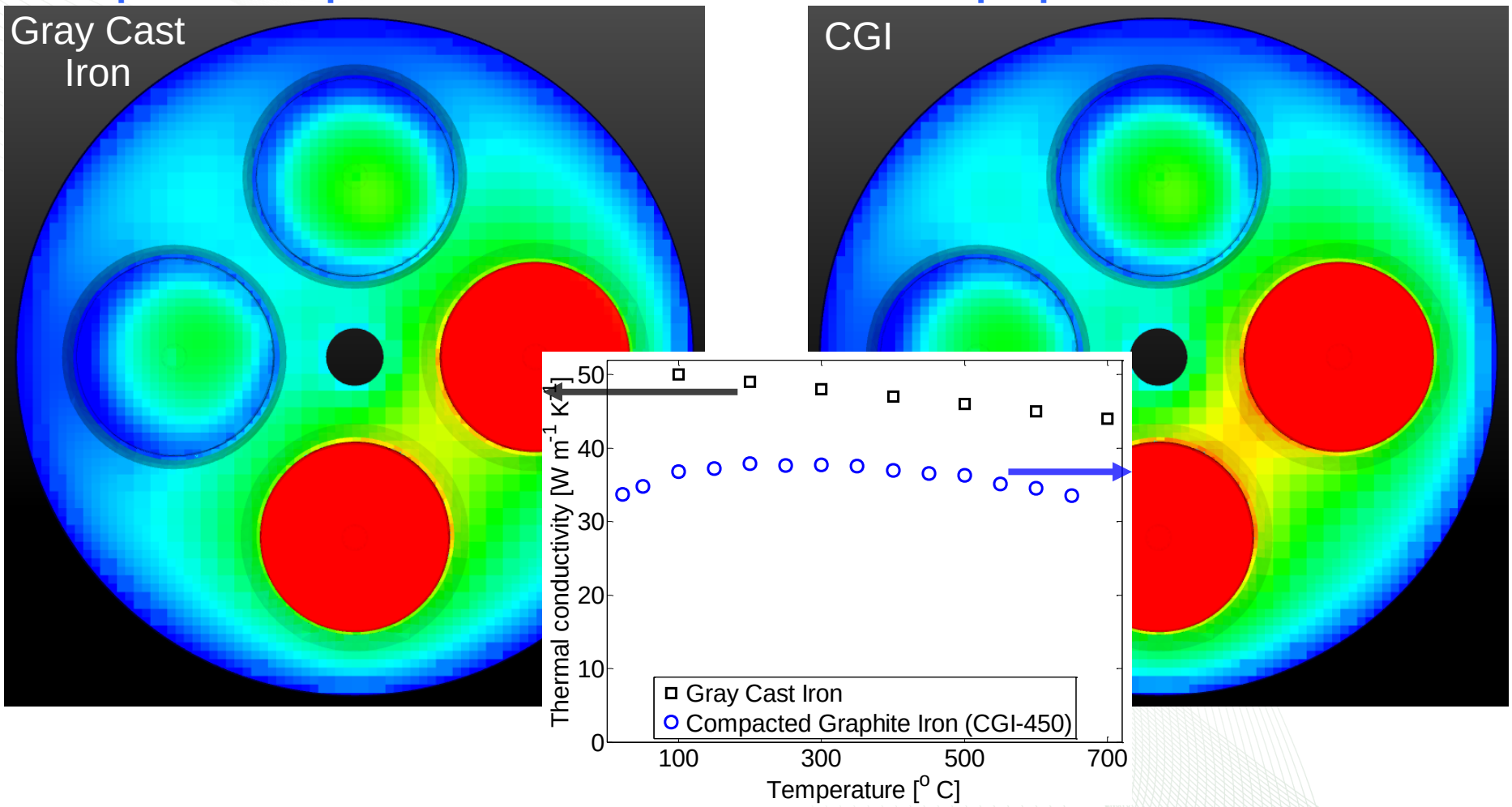
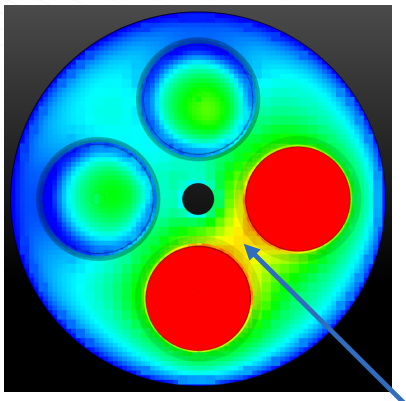
Advanced simulations are in progress, evaluating materials effects on temperature, heat flux, and combustion

Component temperatures are function of materials properties and combustion

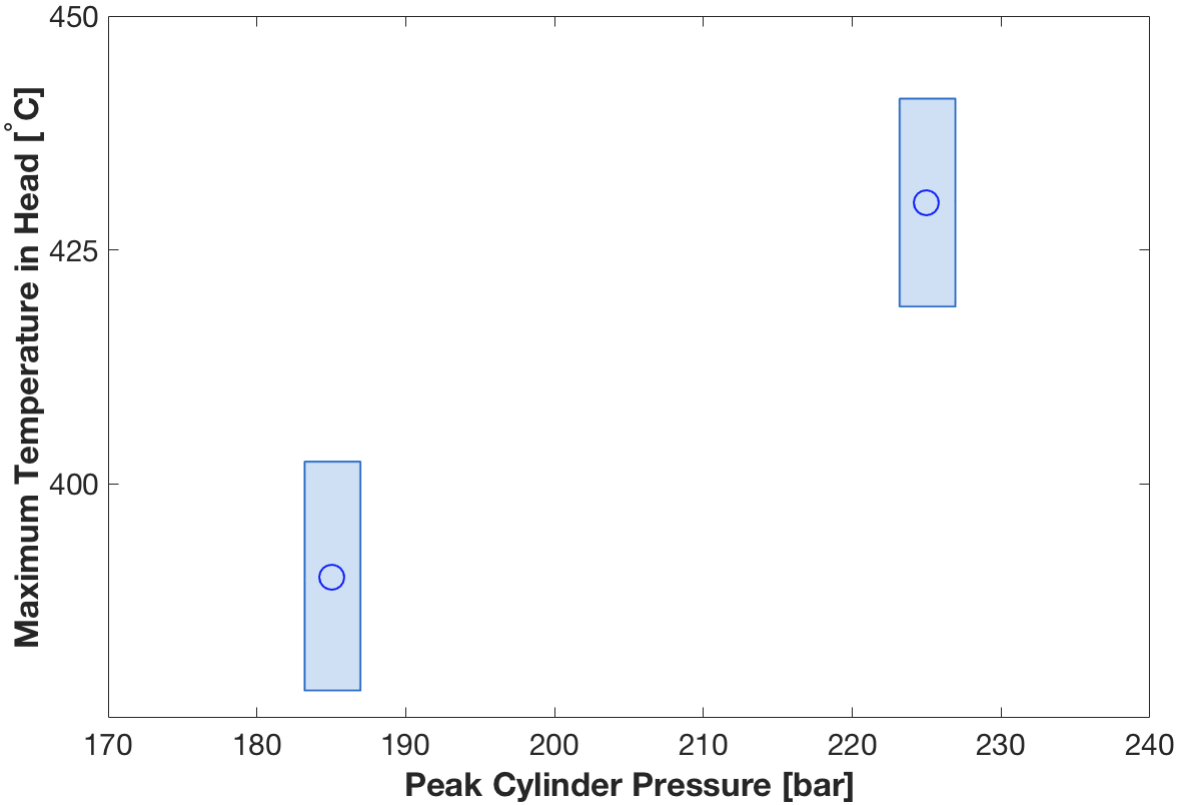


Early simulation results suggest materials will be stressed at higher specific-power operation

Higher pressures and gas temperatures with increase in specific power raise materials temperatures



Highest head temperatures in bridge between exhaust valves



Preliminary results based on coarser resolution simulations.
Steady-state operation, not accounting for engine transients.

TECHNICAL ACCOMPLISHMENT

Future work will extend methods to other domains

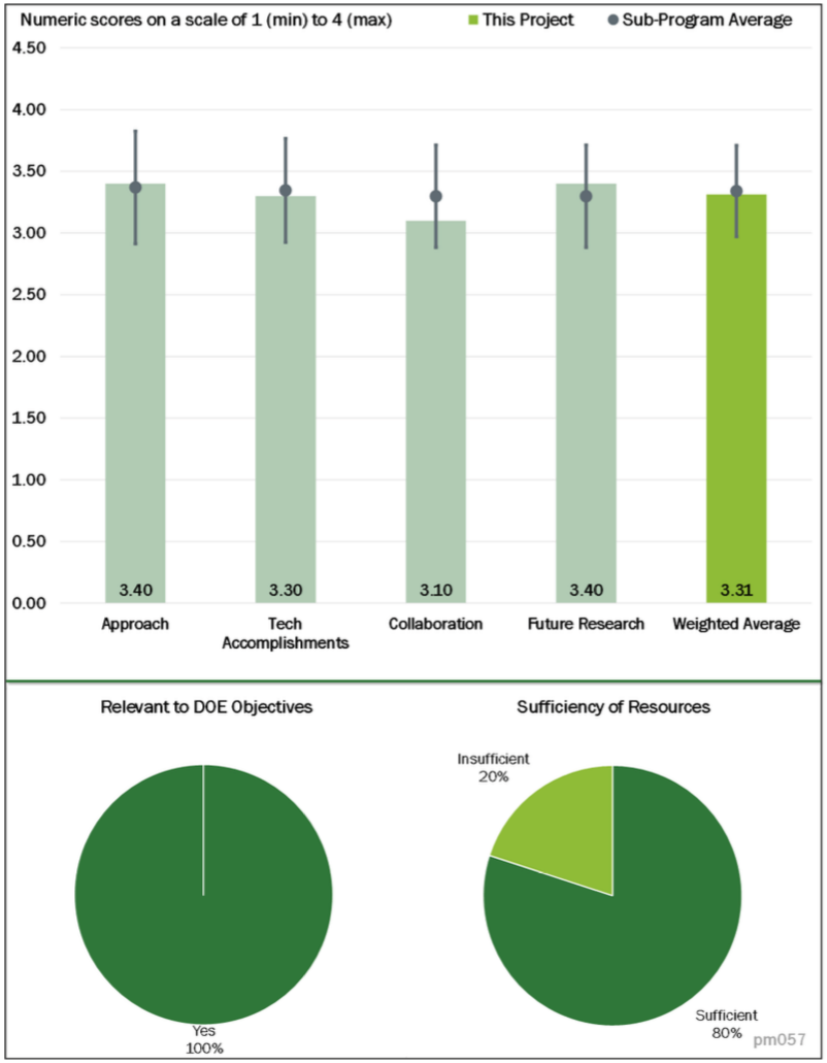
- C**omplete heavy-duty engine study**
  - Complete experimental creep and fatigue studies for CGI-450
  - Continue trajectory of increased specific power
- Implement and validate fully coupled CFD-FEM tools to improve accuracy and flexibility of simulations

  ➔ Non-trivial problem – most fully coupled simulations have operated on single small components (e.g., exhaust manifold, turbocharger assembly)

  ➔ Application for HPC

- **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: Assumption of specific PCP targets may be incorrect (e.g., 300 bar is too high). Response: We are now focusing on increasing specific power, with attendant higher temperatures and pressures, up to the materials limits. Then, the necessary materials properties may be defined for operation beyond those limits.
- Comment: Efforts should be closer tied to OEM needs and experimental knowledge base and not be purely computational. Response: We couple our experiments on materials properties with simulations driven by OEM design and operating data. While we are trying to develop a methodology independently, we will attempt to consult more with OEMs regarding specific strategies for future operation.
- Comment: Collaborations should be more explicitly stated. Response: We mention the degree of collaborations but not specific names or roles to protect sensitivities of some collaborators.

Summary

Contact:
Allen Haynes
haynesja@ornl.gov

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 scoping needs with higher specific-power operation
- Progressed on state-of-the-art co-simulation of combustion and materials thermal properties
- 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 materials properties for future HD engine operation to meet lifespan needs
- Evaluate needs for LD engines utilizing tools developed for HD engines

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