Applied Computational Methods for New Propulsion Materials (PM057)

Task 4: **Future engine requirements**

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Propulsion Materials

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Project Organization

Project encompasses 5 tasks applying various computational methodologies.

Tasks	Budget
1. Catalyst materials	$150 K
2. Permanent magnet materials	$140 K
3. Piezoelectric materials	$100 K
4. HD engine materials requirements	**$140 K**
5. Materials characterization & evaluation	$100 K
	$630 K

◄ Today's review

Task 4 FY2016 Milestone	Due/Status
Complete evaluation of heavy-duty engine materials analysis methodology for fatigue life using properties of current and advanced materials as well as estimation of future materials properties, and determine utility for further application of approach to heavy- and light-duty engine systems	Q4 – On track

Project Overview

Timeline

- **Project start – Q3 FY2014**
- **Project end – Q4 FY2017**
- **Complete – 50%**

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"

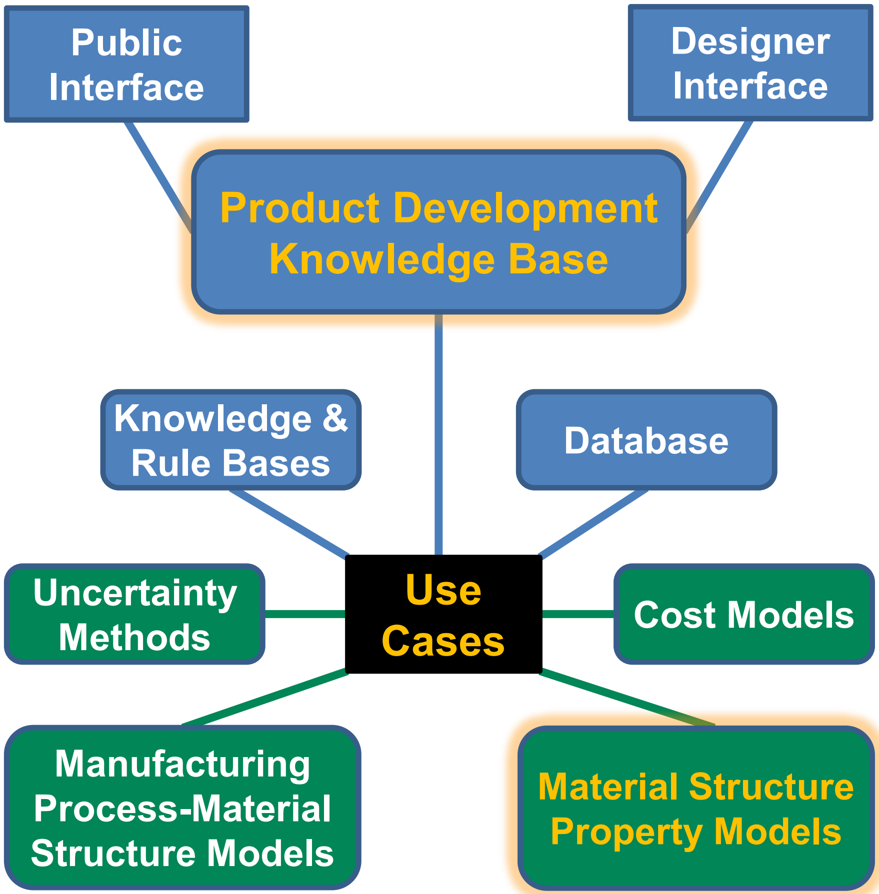
Budget

- **FY2014 – $250 K**
- **FY2015 – $250 K**
- **FY2016 – $140 K**

Partners

- **Cummins, Inc.**
- **Convergent Science, Inc.**

Integrated Computational Materials Engineering accelerates materials development

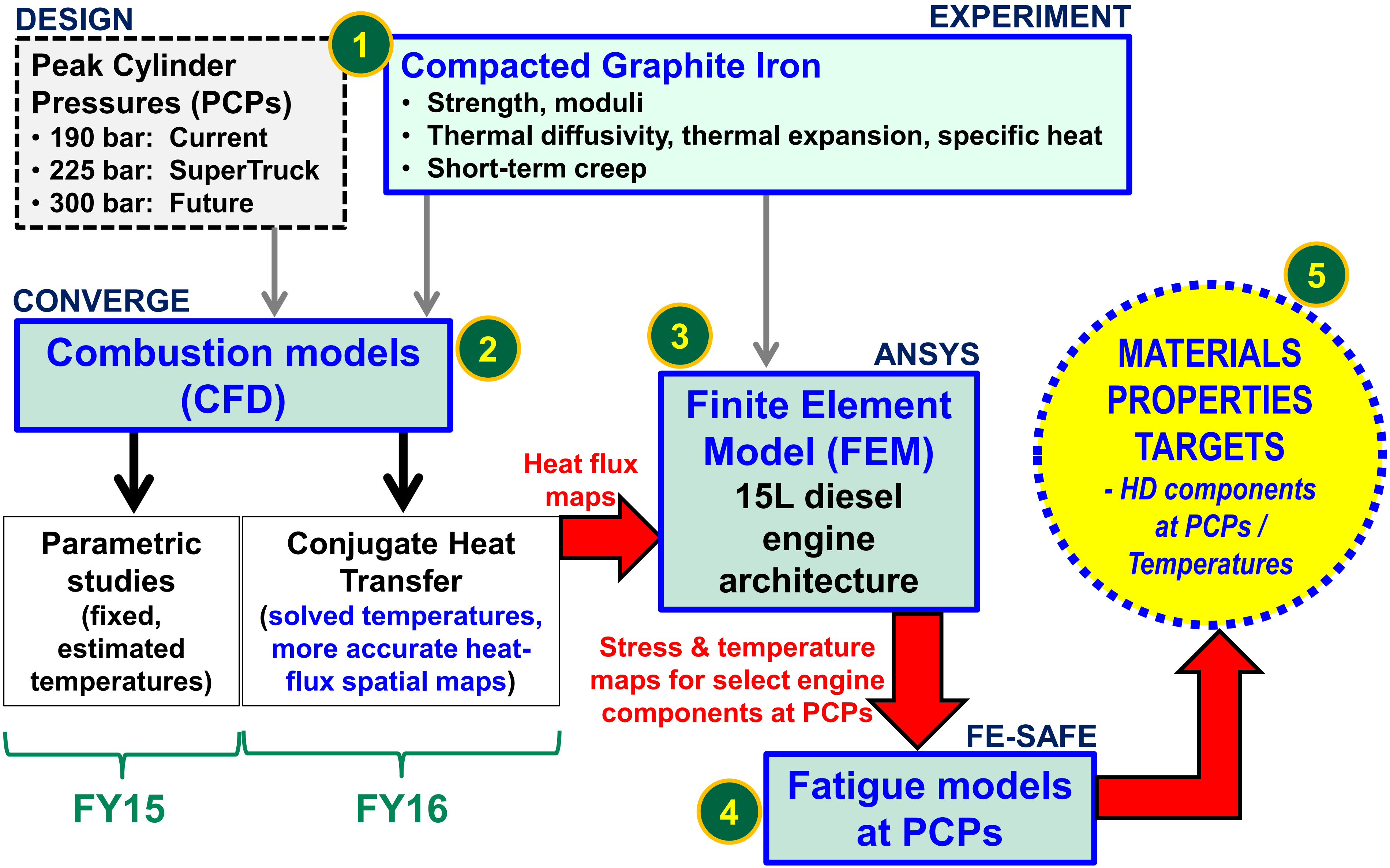


Schematic structure of an ICME system, after Fig. 1-1 in "Integrated Computational Materials Engineering", NAS Press (2008).

- Driver (Barrier): Materials development enables new technologies, but is **slow** and **expensive** – need more efficient approaches (Materials Genome Initiative, OSTP).
- Synergy between modeling & experimental validation is key.
- Goal: Make materials development …

  Faster
  Cheaper
  Less Risky

Integration of experiment and modeling



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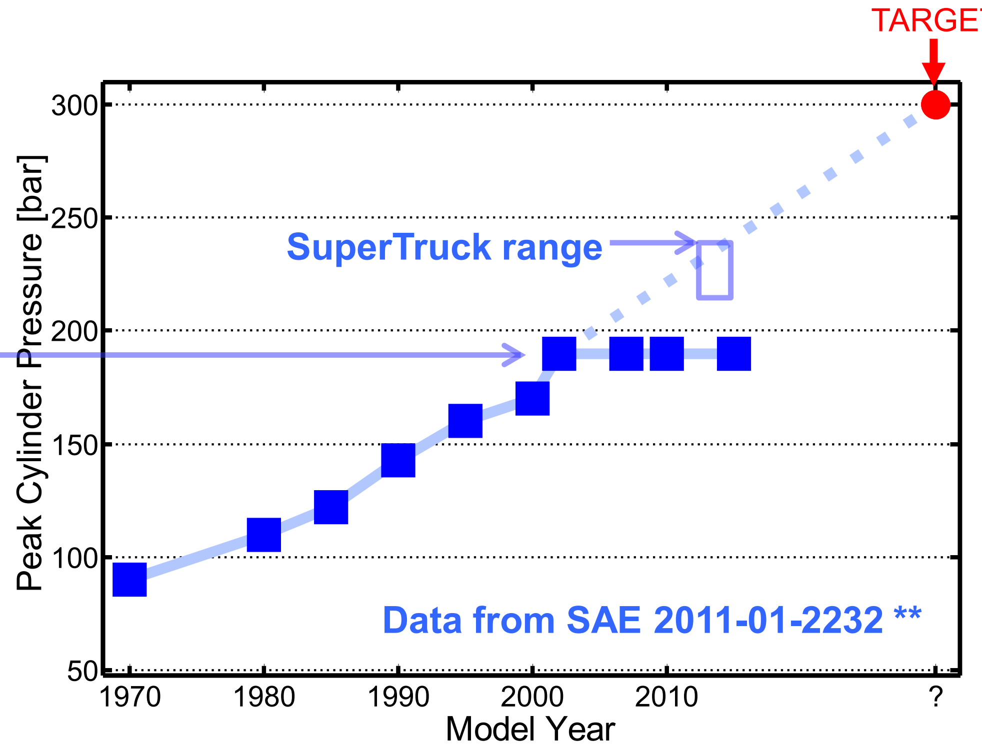
Enabling higher-efficiency engines

RELEVANCE

- Multi-Year Program Plan* Task: Evaluate and characterize emerging materials for application in advanced high-efficiency heavy truck engines
- Roadmap for heavy-duty engine operation projects increasingly **higher peak cylinder pressures** (PCP) and **temperatures** into the foreseeable future to meet efficiency targets
  - SuperTruck programs demonstrated >50% BTE with ≈225 bar PCP, for limited operating spans.
  - 300 bar PCP is long-term goal.

Materials limit heavy-duty production engine peak cylinder pressure

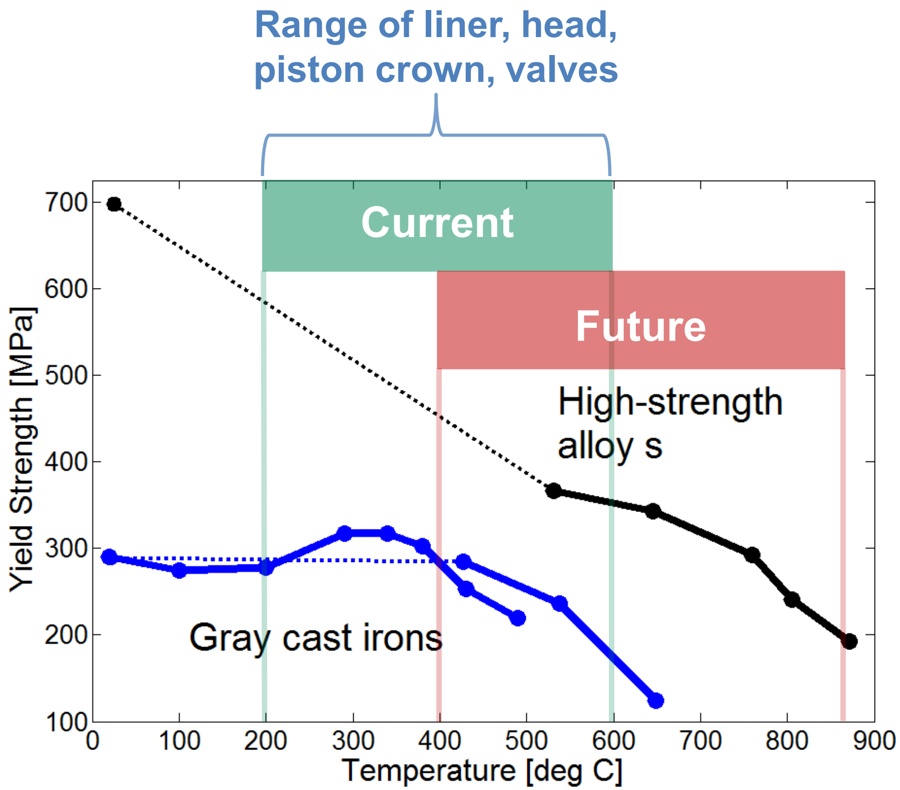


* Vehicle Technologies Program Multi-Year Program Plan (2011-2015).
** M. Megel *et al.* SAE 2011-01-2232; *SAE Int. J. Engines* **4**(3).

Enabling higher-efficiency engines

- Current materials are inadequate for future engines at 250-300 bar
  - Gray Cast Iron is commonly used but considered inadequate.
  - Compacted Graphite Iron is state of the art but not fully evaluated.
  - Materials properties typically **degrade with temperature**, compounding the problem.
- Fatigue life is a concern.
- Creep could be a concern.
- Significant cost constraints.

Material strengths decrease with temperature



Objectives and Approach

Objectives

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

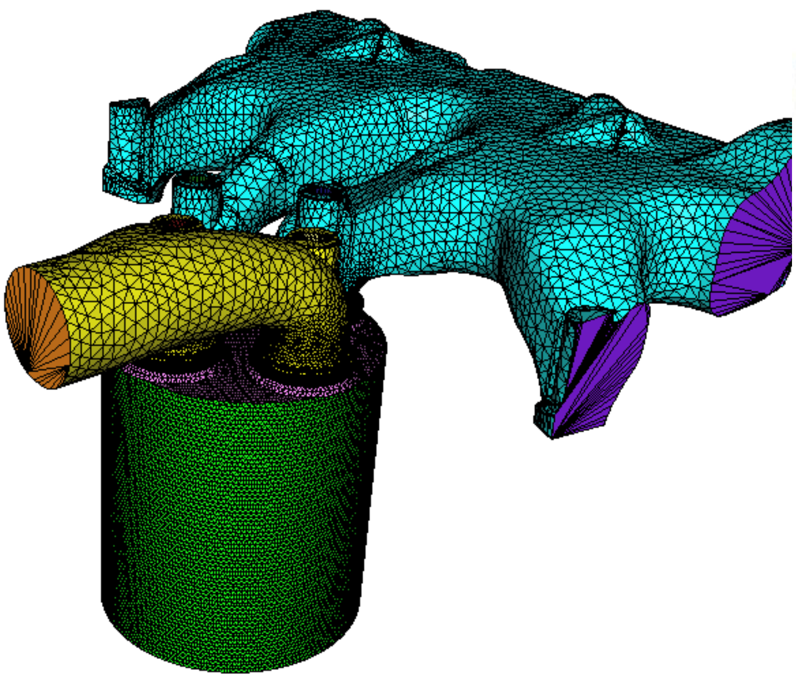
Approach

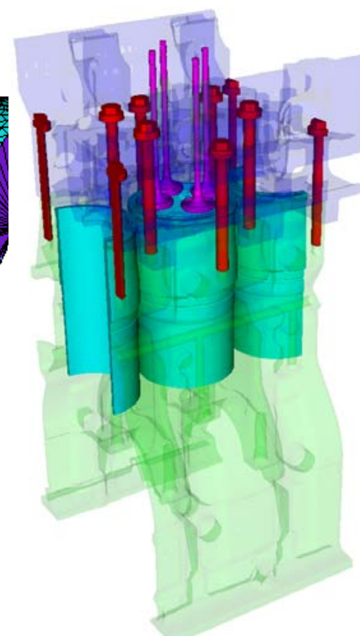
- Use combustion Computational Fluid Dynamics (CFD) modeling to estimate the thermal environment at current and future PCP operating points.
- Use Finite Element Modeling to evaluate effects of pressure and thermal environment on engine cylinder components of interest: **head**, **valves**, **liner.**
  - Initial work (FY14-15): Focus on yield strengths mapping temperature & stresses of current materials (Gray Cast Iron)
  - Ongoing work (FY16): Finalize combustion modeling and materials characterization; focus on predicted requirements of fatigue properties analysis and factors of safety on advanced (Compacted Graphite Iron) and future engine materials

Modeling Approach

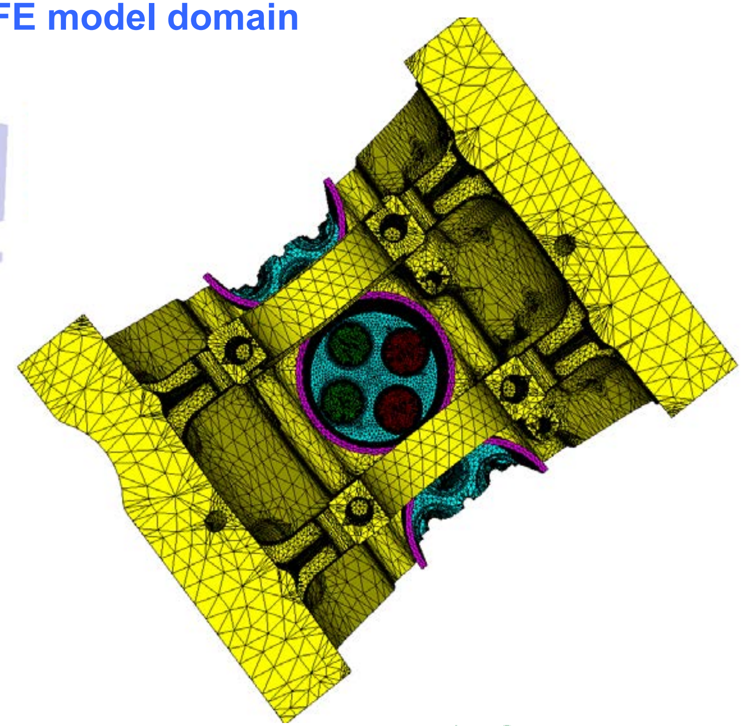
- Apply to modern engines, using established simulation environments
  - Engine: 2013 15-L 6-cylinder engine; focus on single interior cylinder, up to centerlines of neighboring cylinders; based on CAD data
  - Boundary conditions, such as cooling passages and oil splash, defined by known operating conditions/constraints
  - Interfacing industry-standard packages such **CONVERGE** (CFD), **ANSYS** (FEM), and **FE-SAFE** (fatigue)

CFD model domain





FE model domain

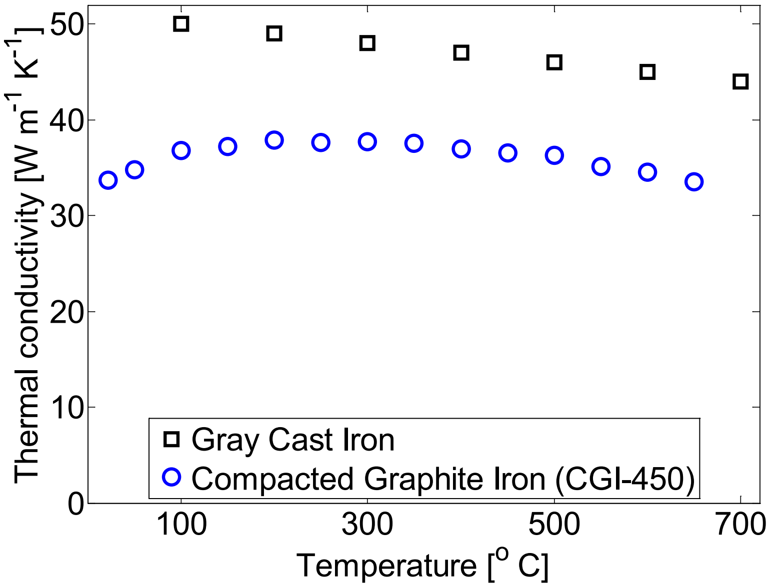


Activities and Progress – Materials characterization

TECHNICAL ACCOMPLISHMENT

- **Experimentally measure relevant properties for Compacted Graphite Iron (CGI-450) at an expanded range of temperatures (up to 650-800 °C)**
  - Tensile strength [complete]
  - Thermal diffusivity [complete]
  - Coefficient of thermal expansion [complete]
  - Critical temperatures [complete]
  - Specific heats [complete]
  - Short-term creep [in progress]

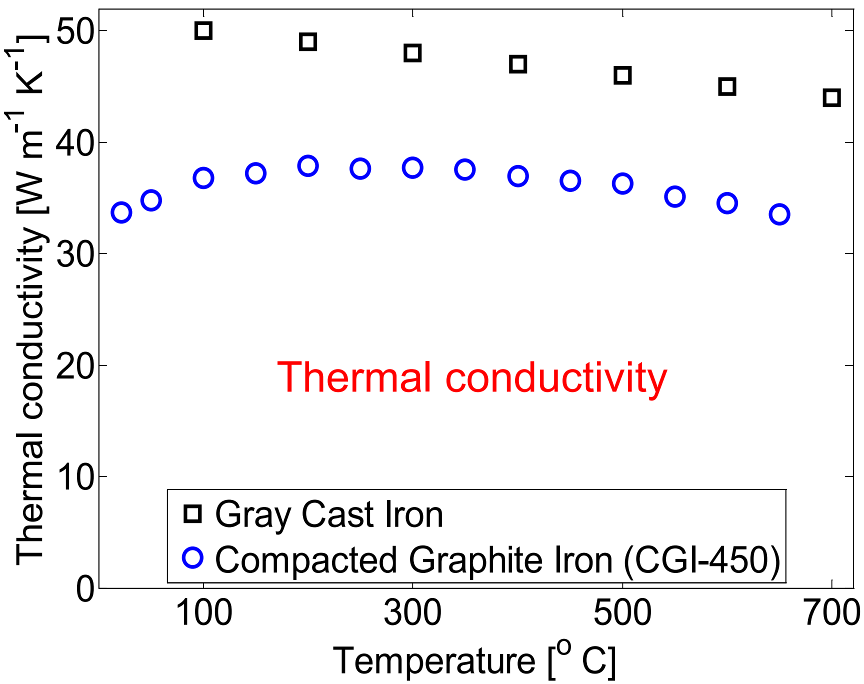
Utility:
- Assists engine-design community
- Supports this project modeling efforts

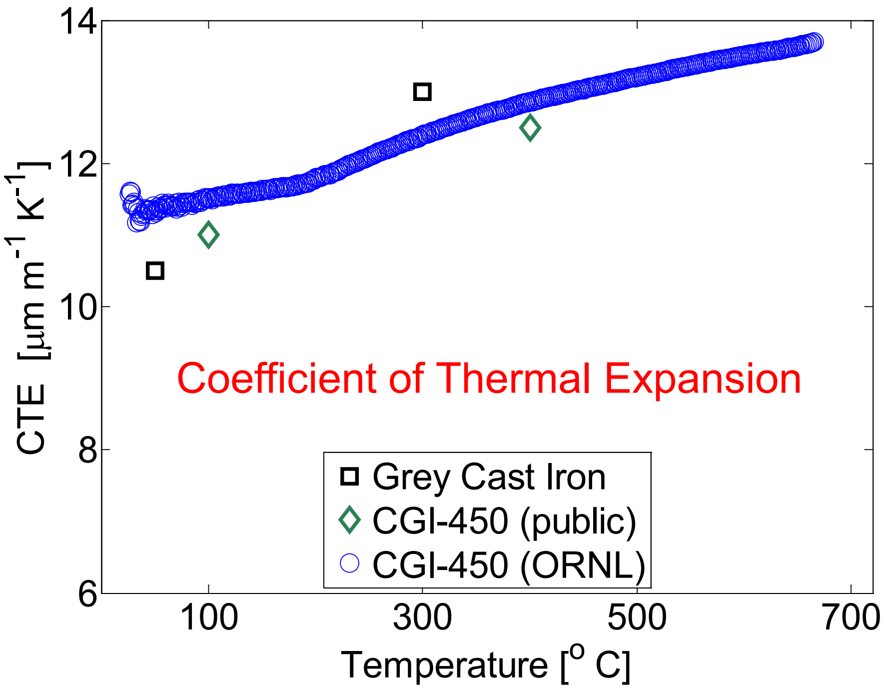


Average experimental thermal conductivity versus temperature of CGI-450, with Gray Cast Iron for comparison

Thermal properties of some commonly used cast irons (CGI-450 measured at ORNL)

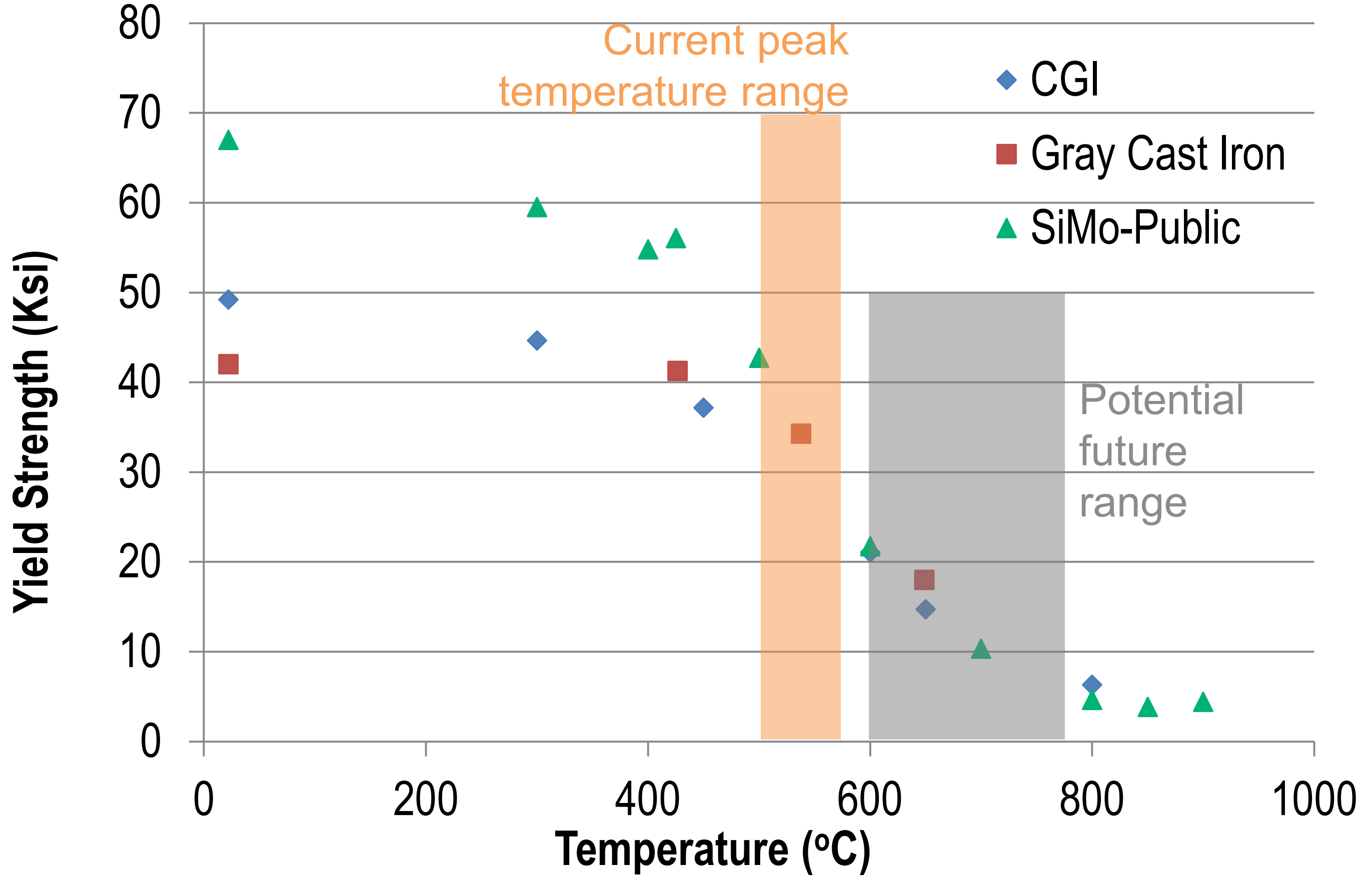
TECHNICAL ACCOMPLISHMENT





Many cast irons have similar tensile properties at elevated temperatures

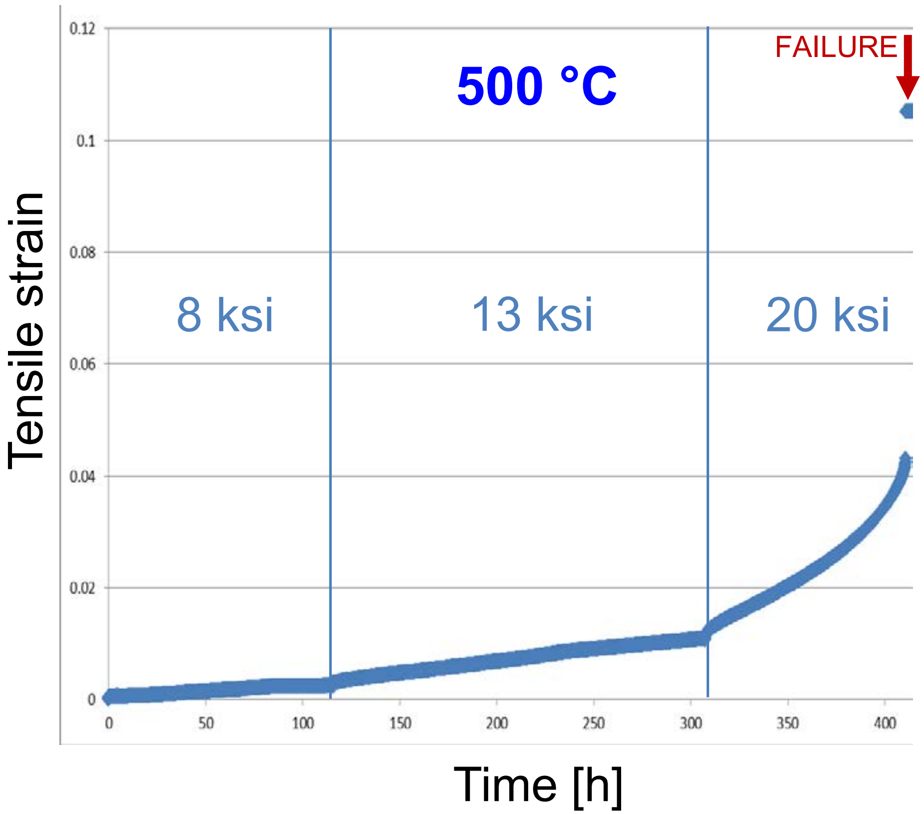
TECHNICAL ACCOMPLISHMENT

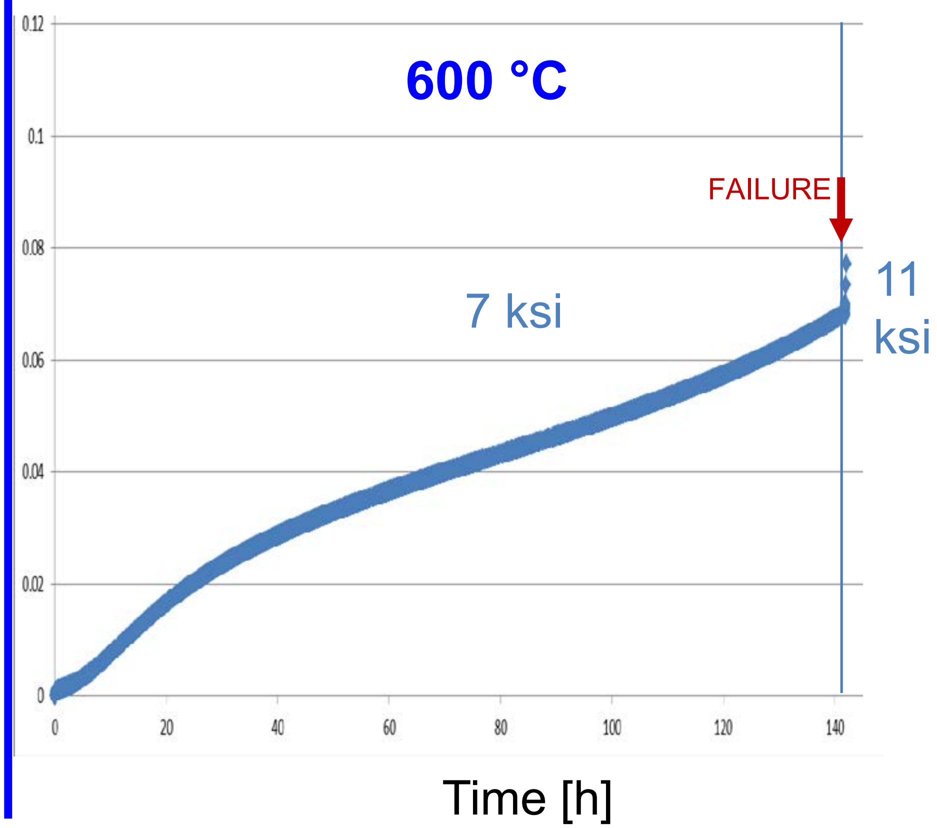


Additional materials characteristics, including fatigue, determine suitability for more severe engine applications.

Short-term step-loading creep tests of CGI-450 are in progress

TECHNICAL ACCOMPLISHMENT





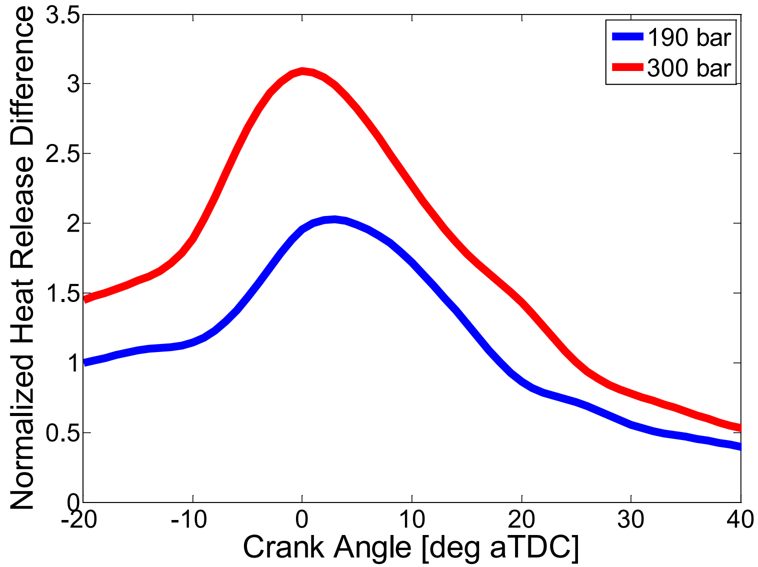
Activities and Progress – Combustion modeling

TECHNICAL ACCOMPLISHMENT

- **Parametric studies with imposed surface temperatures, to gage effects of surface temperatures, exhaust gas recirculation, etc. and evaluate other heat transport effects [FY15,FY16]**
- **Conjugate heat transfer (CHT) modeling to solve combustion and materials temperatures iteratively, for accurate thermal spatial distribution [FY16]**
- **Tuning CHT model for three PCP conditions: 190 (current practice), 225 (SuperTruck range), 300 bar (future target).**

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

Effects of 100 K uncertainty in imposed surface temperature on heat transfer at two PCPs



Computational heat-transfer strategies

Motivation: Accurate materials temperatures are crucial for combustion and thermo-mechanical stress analysis

Imposed-temperature heat transfer

- Estimate surface temperatures
  - Little measured data available at these conditions
  - Combustion and heat flux from cylinder through materials less accurate
- How far off will estimates at 300 bar be?

Conjugate heat transfer (CHT)

- Co-solve gas and materials temperatures
- Temperature and heat-flux distribution more accurate than imposed-temperature solutions, especially with localized variations (e.g., valve bridges)
- Slower simulation (~3-4 times longer per case) and more resource intensive

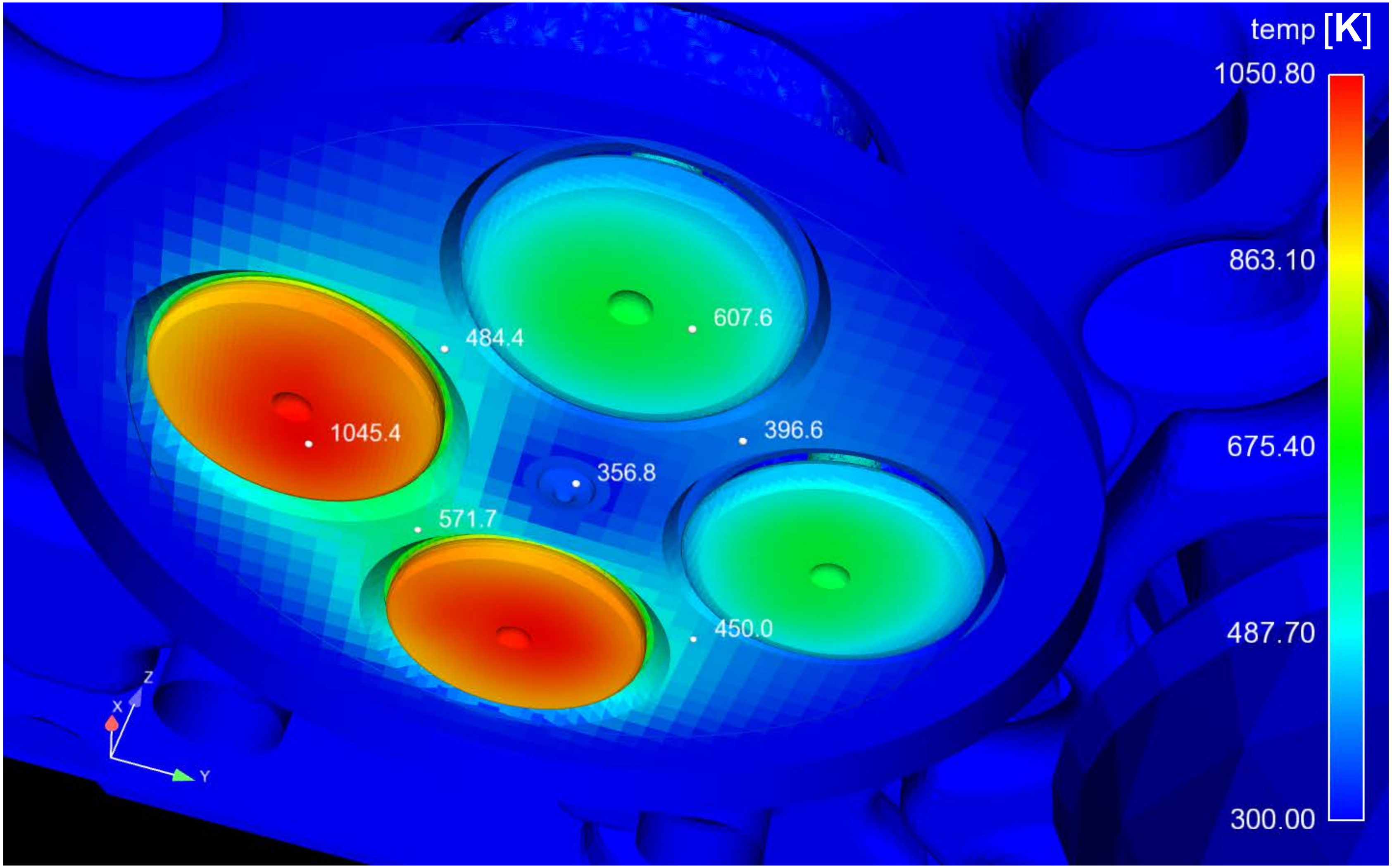
CHT is most rigorous way to model extreme PCP conditions, including 300 bar.

Simulations with CHT are ongoing to permit better prediction of thermal conditions at elevated pressures and temperatures.

CHT simulations are in progress

TECHNICAL ACCOMPLISHMENT

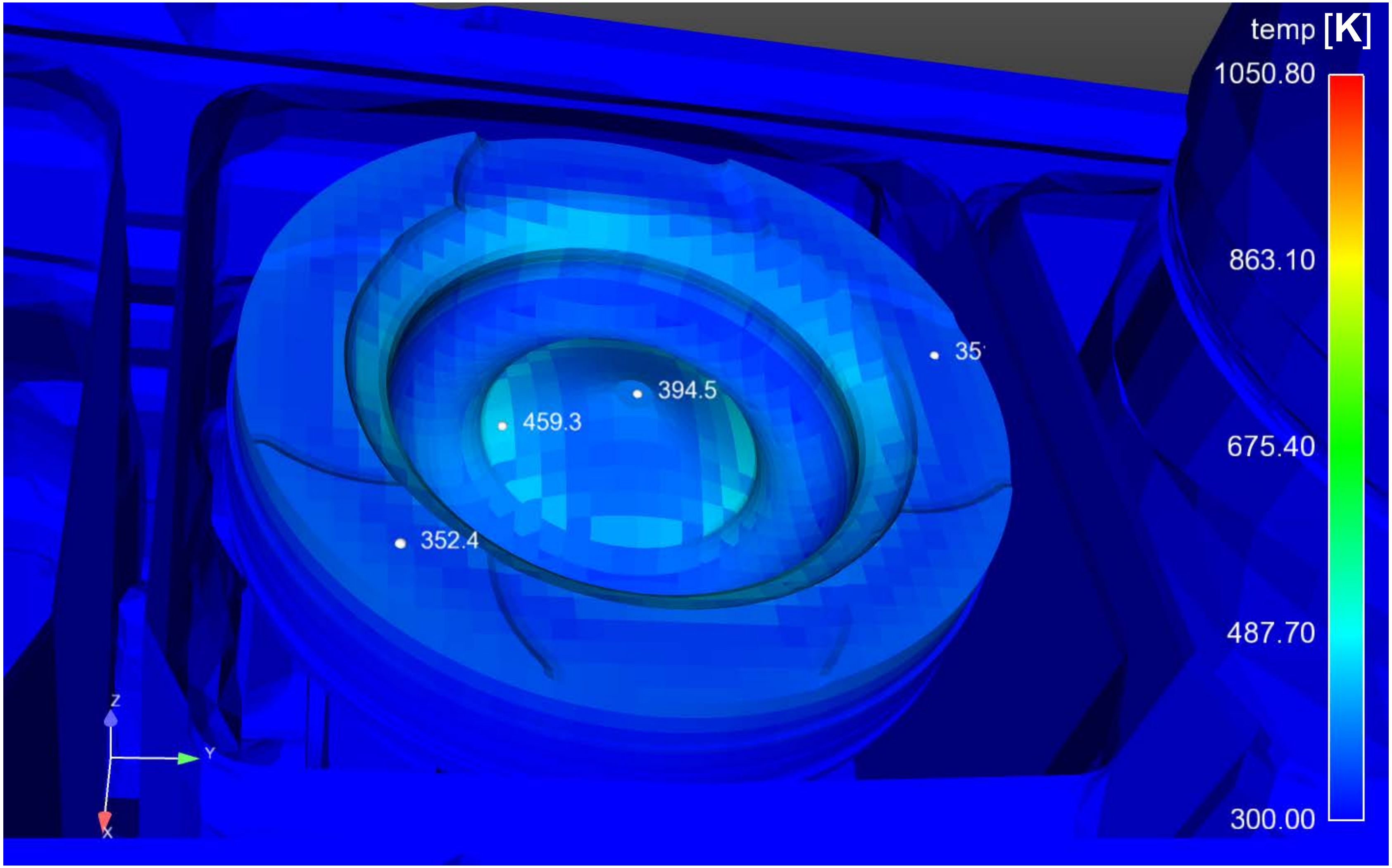
Head temperature distribution at low-PCP condition



CHT simulations are in progress

TECHNICAL ACCOMPLISHMENT

Piston crown temperature distribution at low-PCP condition



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Future research

FUTURE WORK

FY16

- Continue tuning CFD with CHT at all target PCP
- Integrate CFD results into FEM analysis
- Develop analysis methodology for fatigue life using properties of current and advanced materials as well as estimation of future materials properties

FY17

- Predict fatigue behavior at all PCPs for grey cast iron and CGI and predict necessary materials properties for future engines at extreme PCPs
- Further refine methodology and determine utility for further application of approach to heavy- and light-duty engine systems

Future

- Implement 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)

- Extend methodology to light-duty engines – higher-temperature but lower service life environment with lower cost margins

Responses to Prior Year Comments

- **Reviewer comments: While it may be valuable and novel to incorporate CFD in this task, the reviewer went on, it does not utilize the principles of ICME significantly (i.e., multiscale integration). However, the coupled approach (CFD and FEM) appeared to the reviewer to be sensible and useful no matter what it is called. The reviewer considered that a much more thorough explanation of the intended limited goals would be appropriate, along with a concerted presentation of the next steps with an emphasis on the critical areas to study next.**
  – We agree that this specific task, at its present stage of implementation, does not utilize multiscale integration implicit in ICME. Our project title now reflects an emphasis on applied modeling methodologies. We hope that the utility of coupling CFD and FEM will become more apparent as we are able to evaluate materials performance and future needs. We have attempted to be more descriptive of our approach and objectives with this year's report.
- **The reviewer characterized the team of collaborators as consisting of several well-qualified institutions, but saw very little discussion of how these collaborators are contributing to the project. More specifically, the reviewer said it was unclear which collaborators are directly contributing to Task 4, the subject of this presentation.**
  – We agree with this observation and will address it in the future where possible. There are some cases where partners are involved and willing to be acknowledged, but do not want their specific role publicly described. In those cases, we will have to continue to be non-descriptive.

Summary

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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

- Implemented state-of-the-art co-simulation of combustion and materials thermal properties
- Implemented coupling of CFD and FEM for specifying future materials needs
- Completed 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 HD engine operation at 300 bar to meet lifespan needs
- Evaluate needs for LD engines