Oak Ridge National Laboratory

Modeling of Light-Duty Engines*

* Subtask 4B4 under the Powertrain Materials Core Program (PMCP)

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Oak Ridge National Laboratory

2020 U.S. DOE Vehicle Technologies Office
Annual Merit Review

June 4, 2020

Project ID: **mat186**

<u>Program</u> Overview: VTO Powertrain Materials Core Program

Timeline/Budget

- Lab Call Award: July 2018
- Budget: $30M/5 years
- Program Start: Oct 2018
- Program End: Sept 2023
- 30% Complete

Barriers

- Increasing engine power densities & higher efficiency engines; resulting in increasingly extreme materials demands (increased pressure and/or temperature)
- Reducing emissions in ICEs (by elevating engine efficiency)
- Affordability of advanced engine materials & components
- Accelerating development time of advanced materials
- Scaling new materials technologies to commercialization

FY20 Program Research Thrusts	FY20 Budget	Participating Labs
1. Cost Effective LW High Temp Engine Alloys	$1.05M	ORNL
2. Cost Effective Higher Temp Engine Alloys	$1.525M	ORNL, PNNL
3. Additive Manufacturing of Powertrain Alloys	$1.075M	ORNL
4A. Advanced Characterization	$1.025M	ORNL, PNNL, ANL
4B. Advanced Computation	**$0.60M**	**ORNL**
5. Exploratory Research: Emerging Technologies	$0.75M	ORNL, PNNL, ANL

Partners

- Program Lead Lab
  - Oak Ridge National Lab (ORNL)
- Program Partner Labs
  - Pacific Northwest National Lab (PNNL)
  - Argonne National Lab (ANL)

Program structure includes three alloy development thrusts (1-3), a foundational support thrust (4), and a thrust for one-year exploratory projects (5).

Project Overview: Subtask 4B4 (Modeling of Light-Duty [LD] Engines)

Timeline/Budget

- Project start: Oct 2019
- Project end: Sep 2022
- Percent complete: 22%
- **Subtask 4B4 Budget**
  - **FY19: $0k**
  - **FY20: $150k**

Barriers

- Need prediction of internal combustion engine (ICE) operating conditions as engine power densities further increase.
- Need prediction of effects of future, higher-efficiency engine combustion regimes on materials in specific components and definition of the set of needed materials properties.

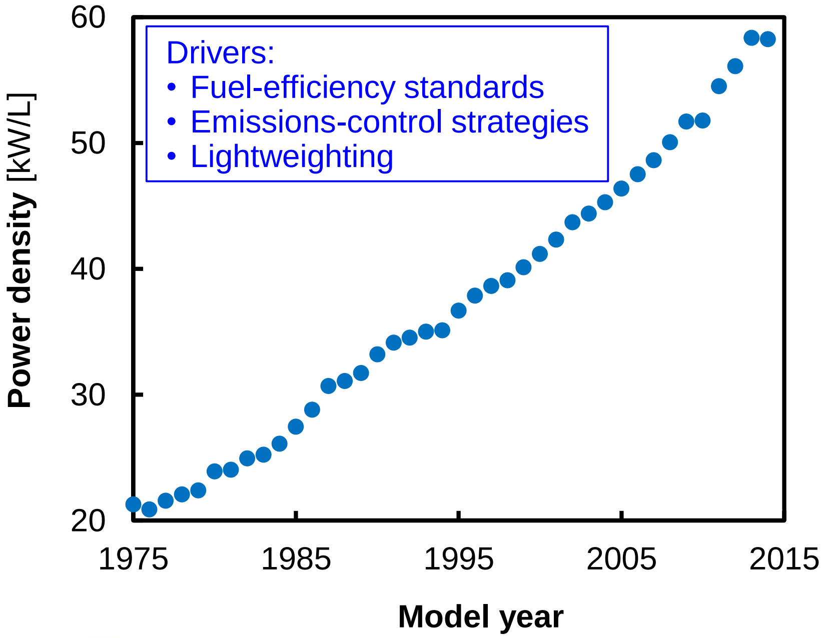
Thrust 4: Tasks/Subtasks	Lab	PI(s)	FY19	FY20
Task 4A: Advanced Characterization				
4A1: Advanced Characterization	ORNL	Watkins	$450k	$425k
4A2: Advanced Characterization	ANL	Singh	$300k	$300k
4A3: Advanced Characterization	PNNL	Devaraj	$300K	$300k
Task 4B: Advanced Computation				
4B1 – 3: Computational Materials	ORNL	Shin	$450k	$450k
4B4. Modeling of LD Engines	ORNL	Finney	0	$150k

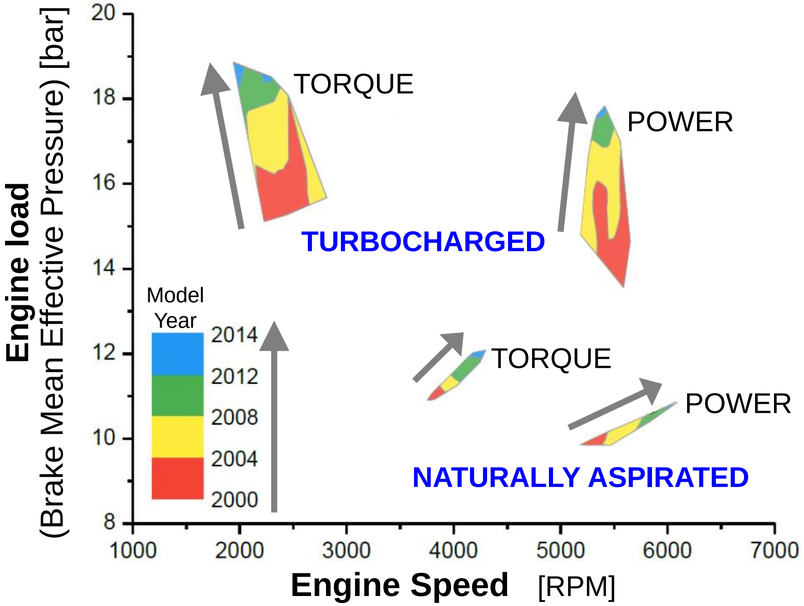
Partners

- 4B4 partners
  - Convergent Science, Inc. (software)
  - Partnership on Advanced Combustion Engines (PACE) – DOE Vehicle Technologies Office

Motivation

- Light-duty engines are increasingly stressed
  - Causes: Increased specific output (torque, power etc) via downsizing/lightweighting
  - Effects: Higher pressures & temperatures → nearing materials temperature limits now
- New materials will enable operation at higher temperatures
  - Reduce need for protective enrichment (adding extra fuel to cool components)
  - Enable further downsizing
  - Permit selective cooling to optimize engine thermal management & efficiency
- Need better understanding of future operating environment to balance efficiency and lightweighting





After Splitter D, Pawlowski A, Wagner R (2016). *Frontiers in Mechanical Engineering* **1:** 16. DOI https://doi.org/10.3389/fmech.2015.00016.

Milestones

Milestone	Description	Due date	Status
Q1	Construct LNF engine system model in GT-Power integrating scanned geometries for heat-transfer modeling	December 31	COMPLETE
Q2	Construct combustion model in CONVERGE CFD integrating scanned geometries for heat-transfer modeling	March 31	COMPLETE
Q3	Construct finite-element (FE) model in ANSYS using refined scanned geometries with CFD predicted heat fluxes for thermal loading and predicted pressures for mechanical loading	June 30	ON TRACK
Q4	Complete simulations for validated combustion model and refined FE model at a baseline and increased specific output condition	September 30	ON TRACK

Project objectives

DEFINE FUTURE CONDITIONS

Estimate thermal environment of cylinder materials (valves, piston, head) of representative light-duty engines at increased specific output

DEFINE MATERIALS PROPERTIES

Estimate required materials properties at future operating conditions

LEVERAGE DOE RESEARCH

Utilize and integrate with ongoing activities in PMCP* & PACE**

ADVANCE STATE OF THE ART

Make results, methodology, and data available publicly to further the industrial state of the art & help define relevant targets

* Propulsion Materials Core Program, DOE Vehicle Technologies Office

** Partnership on Advanced Combustion Engines, DOE Vehicle Technologies Office

This project integrates several modeling approaches and objectives

SCOPING STUDY

Background study to explore operation limits and strategies enabled by higher-temperature materials*

→ ?

How would better materials enable improved engine efficiency & where is the most opportunity?

* **Eliminate protective enrichment**
Enable further downsizing
Explore selective cooling strategies

INTEGRATED COMBUSTION AND STRUCTURAL STUDY

Combustion modeling to define thermal environment experienced by light-duty engine components at projected future operating conditions

Finite element modeling to predict materials stresses, strains etc based on combustion modeling of projected future operating conditions

→ ?

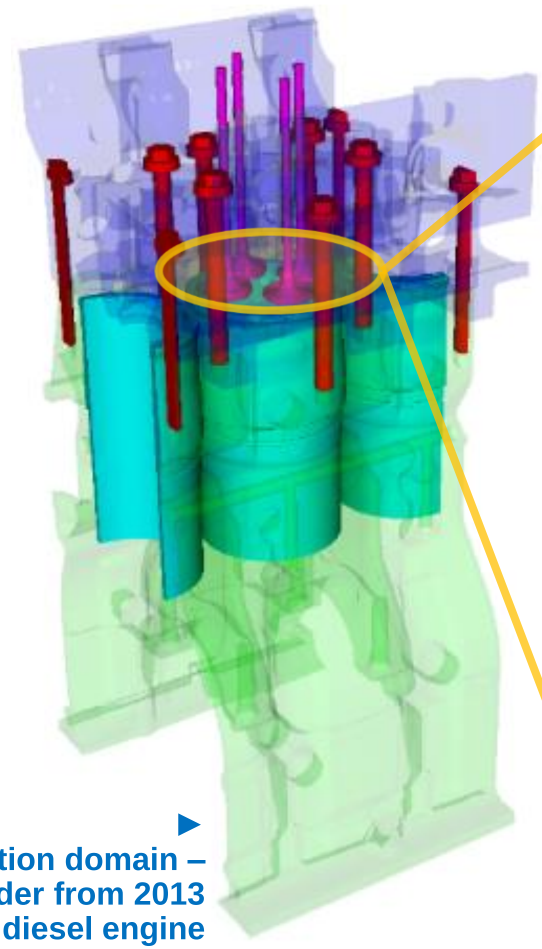
Which materials properties are needed?

Will new fuel formulations require new materials?

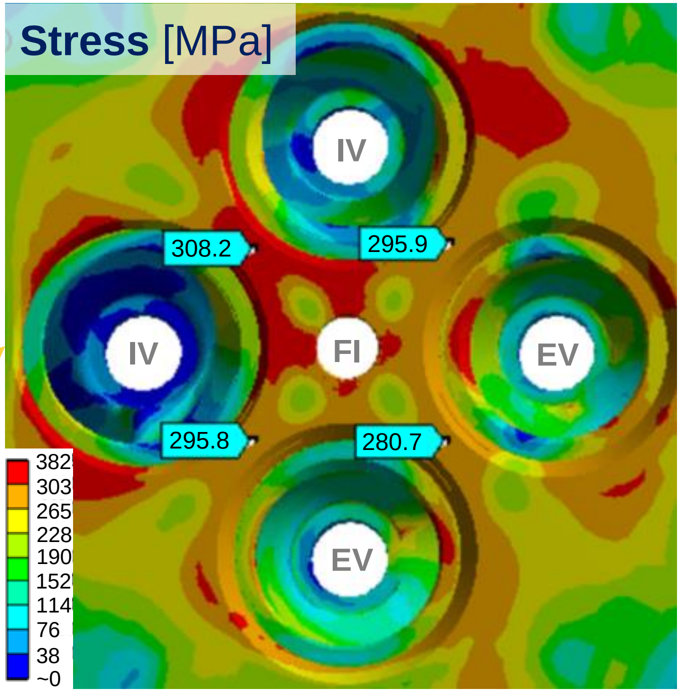
Both studies target modern, production passenger engines run at ORNL & use materials data measured at ORNL.

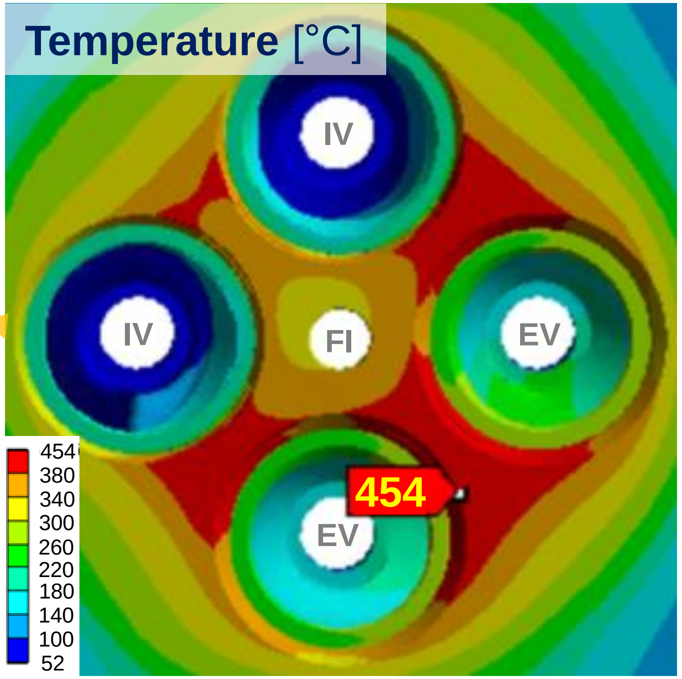
This study follows methodology developed in the materials program for heavy-duty engines

- A recent, prior project explored the effects of increasing power density by 25–50%
- Two industry-standard materials were evaluated to develop methodology: gray cast iron & Compacted Graphite Iron (CGI-450)
- ORNL measured materials properties for CGI-450, extending into higher temperatures than publicly available
- A combined modeling approach used computational fluid dynamics and finite element analysis to estimate the thermal and stress–strain–creep environment
- Results help define roadmap for materials needed for future engine operation



▶ **Simulation domain – single cylinder from 2013 15-L I-6 diesel engine**





▶ **Simulation results – stresses and temperatures in engine head at 25% increased power density**

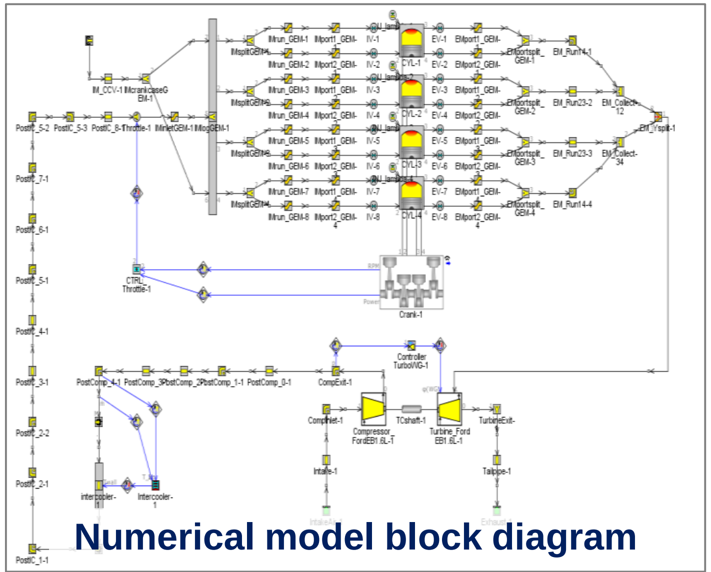
EV: Exhaust valve | IV: Intake Valve | FI: Fuel Injector

Scoping study: explore benefits of different operating strategies enabled by higher-temperature materials

Experimental engine at ORNL for validation data

- 2013 Ford Ecoboost 1.6L 4-cylinder DISI engine
- Single-stage turbocharger
  - Boost levels throttled with wastegate changes
- Stock OEM piston with 9.35:1 compression ratio
- Standard E10 fuel blend with RON of 91
- **Exhaust temperatures limited** to ~900°C, controlled by enrichment

Experimental engine at ORNL



Numerical model block diagram

Numerical model

- GT-Power engine model
  - Base model from Co-Optima
  - **1-D thermal solver for materials temperatures**
  - **ORNL materials data**
- Boost pressures from experimental engine runs
- Turbine maps from OEM
- Combustion & temperature calibrated from experiment
- **Knock model** used to explore practical operating limits with this fuel

Iterative combustion & mechanical modeling

Objective: estimate thermal environment of cylinder materials (valves, piston, head) of engine at increased specific output & define required materials properties

Approach: similar to heavy-duty study from prior years

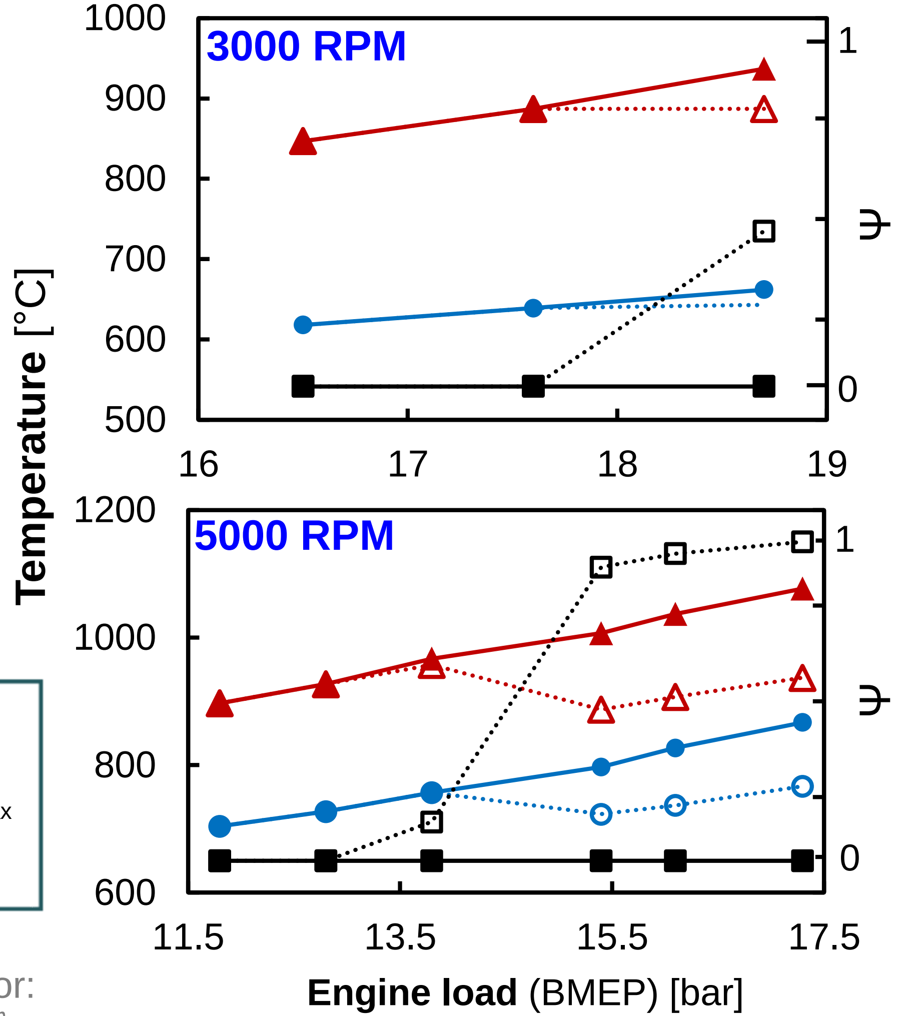
- Experimental approach:
  - Production GM LNF DISI engine at ORNL
  - Design data: high-resolution scans of production head, valves, and piston used for geometry
  - Validation data: ORNL data from PACE — multiple load conditions at 2000 RPM; custom validation data to be taken April–May 2020
- Computational approach:
  - Combustion: GT-Power (0-1D treatment for boundary conditions) and CONVERGE CFD (high-fidelity 3D for spatially detailed heat-flux maps); **conjugate heat transfer** for accurate materials temperatures
  - Structural: ANSYS

Fuel enrichment is used at high engine loads to protect parts

- **Enrichment:** adding extra fuel in order to reduce exhaust gas temperatures - to protect materials from thermal damage
  - Exhaust valves & turbine inlet of primary concern
- Effects of enrichment:
  - $\Delta T_{exhaust\ valve} = -19°C$, $\Delta T_{turbine\ inlet} = -50°C$ at 3000 RPM
  - $\Delta T_{exhaust\ valve} = -46°C$, $\Delta T_{turbine\ inlet} = -110°C$ at 5000 RPM

Enrichment is one strategy to reduce materials temperatures in modern engines at high loads

Component temperatures with engine load, with & without enrichment



Normalized enrichment factor:

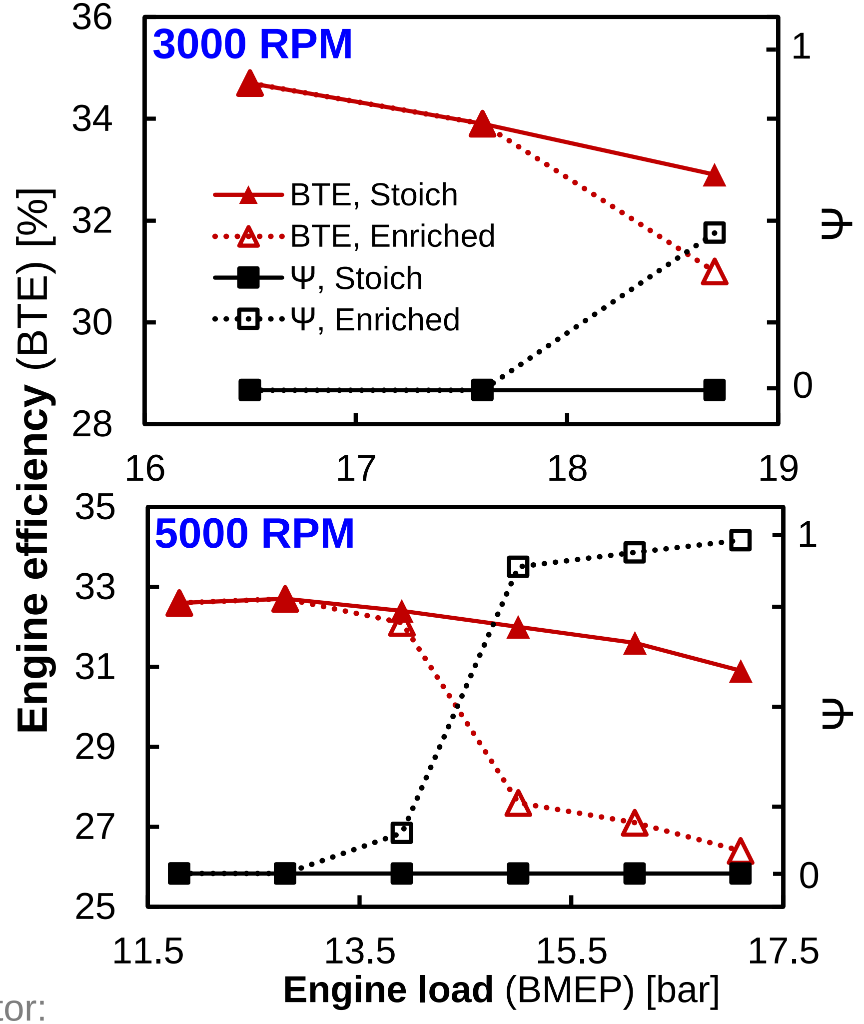
$$\Psi = \frac{1-\lambda}{1-\lambda_{max}}$$

However, enrichment carries a significant fuel penalty

- Large decreases in efficiency are predicted
  - Brake thermal efficiency drops by 1.9% at 3000 RPM, 4.5% at 5000 RPM
  - >10% fuel unburned in worst-case scenario
- Enrichment observed at >75 MPH in some vehicles
- Current engine downsizing trends may necessitate increased enrichment because of the thermal load on materials

Reducing need for protective enrichment with superior engine materials can avoid significant in-use fuel-efficiency and any pollutant emissions penalties

Engine brake thermal efficiency (BTE) with engine load, with & without enrichment

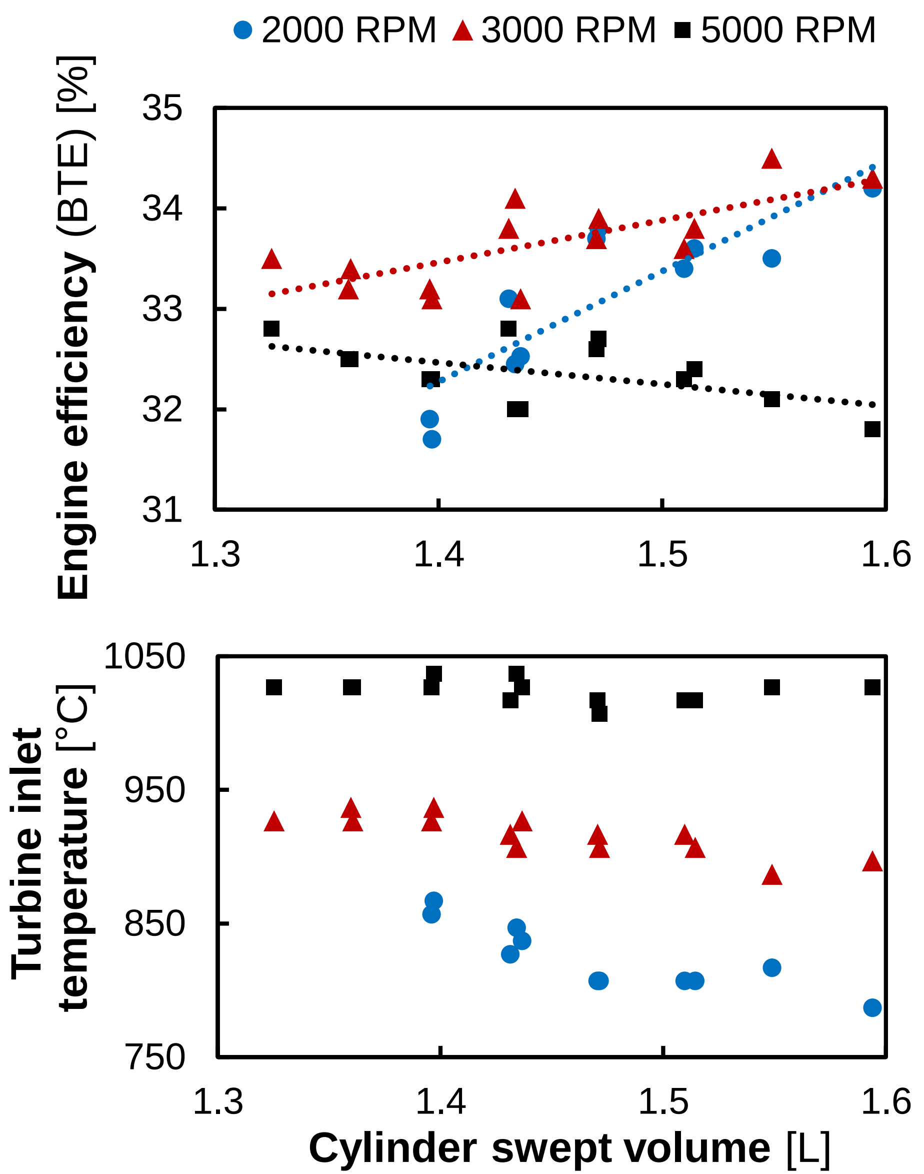


Normalized enrichment factor:

$$\Psi = \frac{1-\lambda}{1-\lambda_{max}}$$

Downsizing provides some efficiency gain but results in higher materials temperatures

- Power held constant while reducing swept volume
  - Stroke: 81.3→75 mm, Bore: 79→75 mm
  - Power maintained with boost (turbocharging)
- ~1% increase in BTE at 5000 RPM from lower frictional losses
- Knock avoidance effects (delaying spark timing):
  - ~2% & ~1% decrease in BTE at 2000 & 3000 RPM
  - Increased exhaust temperatures
  - Turbine inlet temperature increases to 867 °C at 2000 RPM, 937 °C at 3000 RPM, and 1037 °C at 5000 RPM

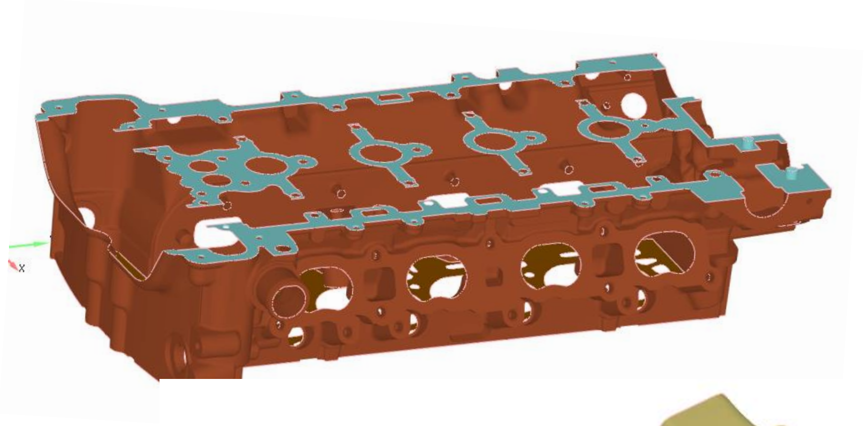


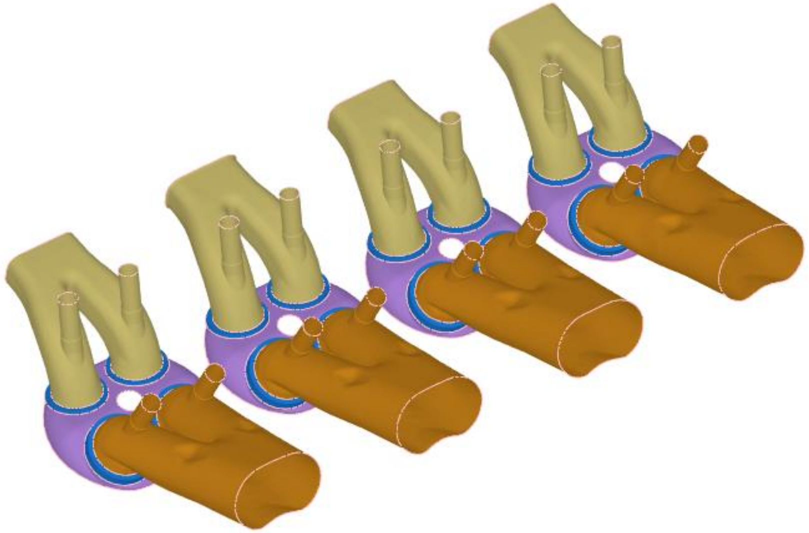
Desired higher power densities will increase materials temperatures significantly

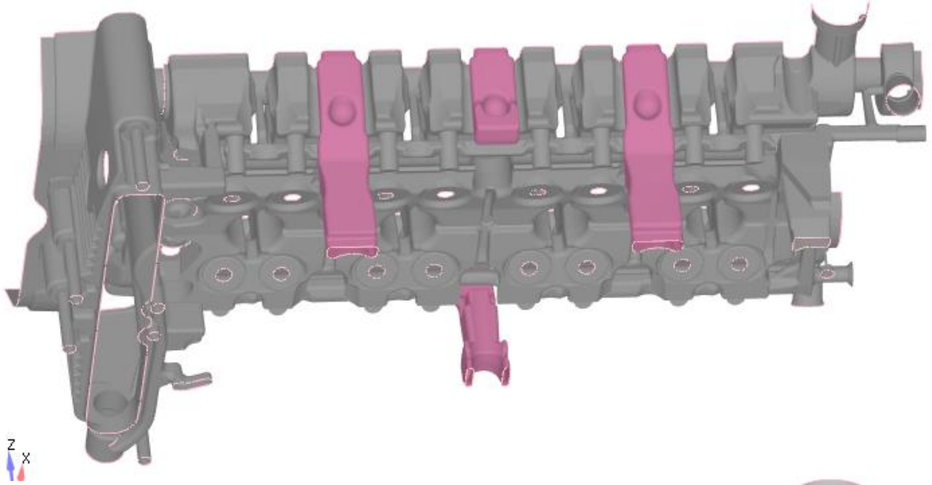
Brake power targets:
44 kW at 2000 RPM
72 kW at 3000 RPM
114 kW at 5000 RPM

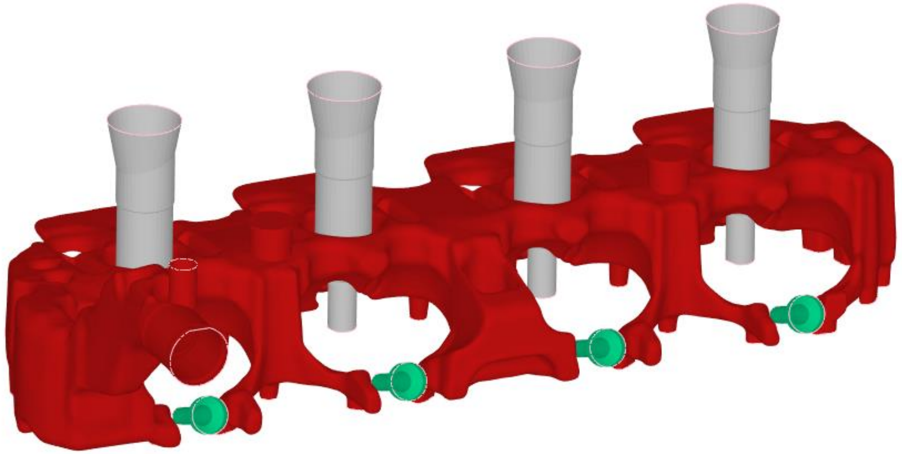
High-resolution scans have been imported into the CFD and FEA models

Some surfaces in the scanned parts need smoothing & simplification for FEA model.
Component surfaces have been separated and tagged for CFD model.





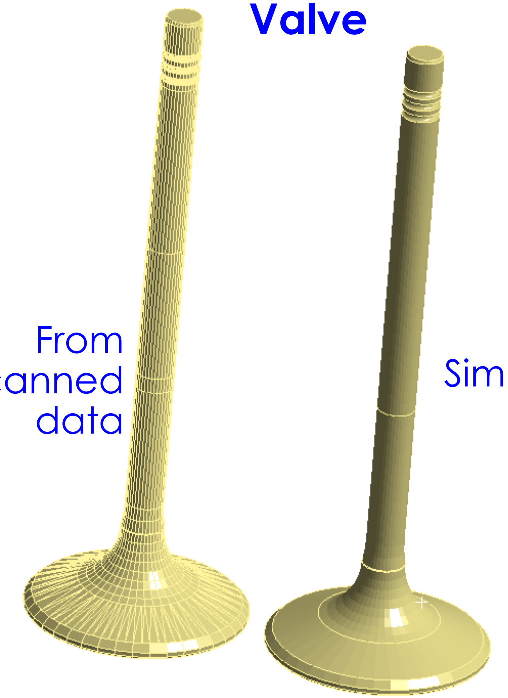




Solid-model simplification for finite element analysis

Physically scanned surface data have been converted to a solid model & are being simplified to reduce computational burden, ease meshing, and improve calculation homogeneity and reliability.

Valve



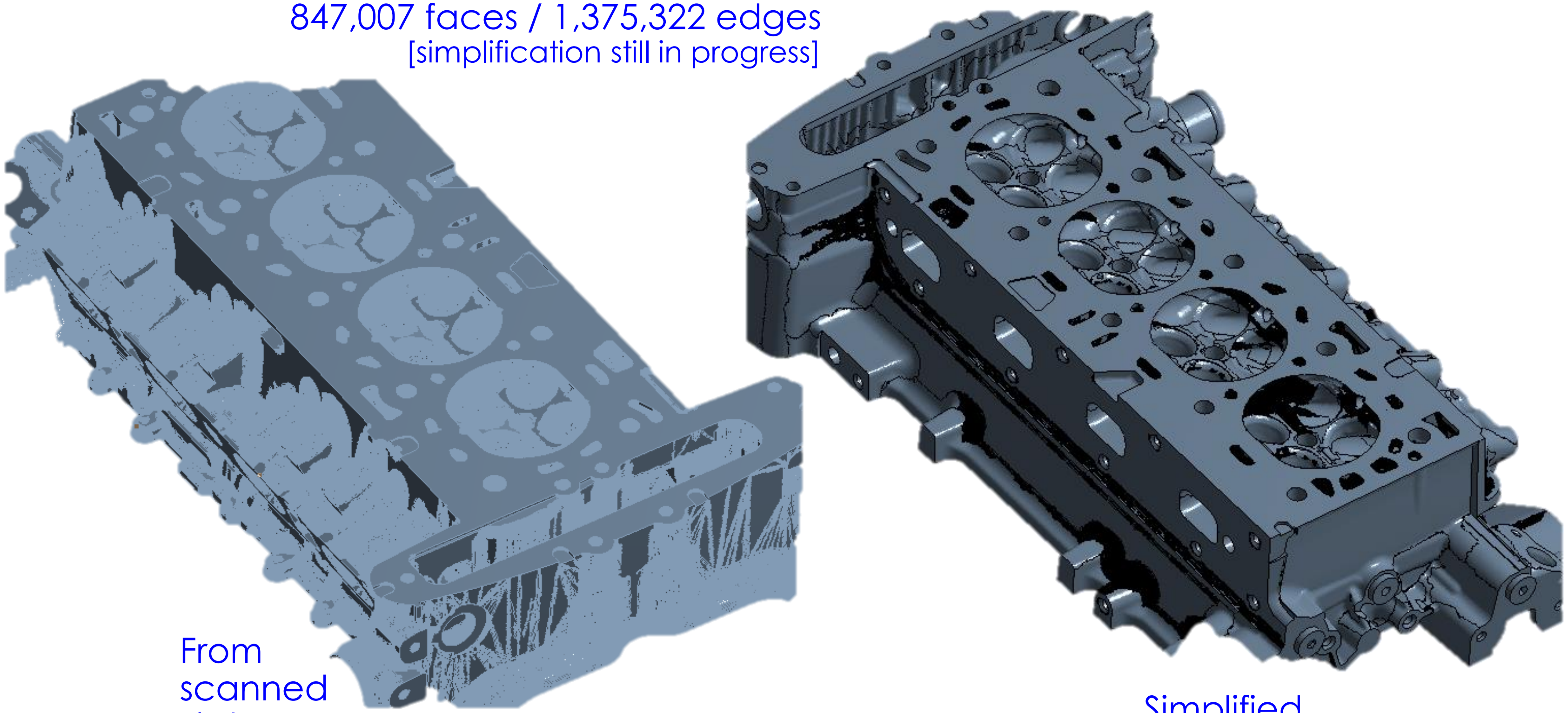
From scanned data

Simplified

3115 faces / 6377 edges to
22 faces / 648 edges

Head

2,228,357 faces / 3,445,279 edges to
847,007 faces / 1,375,322 edges
[simplification still in progress]



From scanned data

Simplified

Current status

Task	Status	Notes/outcomes
LD scoping study (Ecoboost)	COMPLETE	Thermodynamic insights
LD model setup (LNF)	COMPLETE	GT-Power
Q1 Milestone	COMPLETE	GT-Power model setup
CFD model setup (LNF)	COMPLETE	CONVERGE CFD
Q2 Milestone	COMPLETE	CONVERGE model setup
LD model validation (LNF)	IN PROGRESS	Awaiting validation data from PACE tasks
LD model predictions (LNF)	FUTURE	Inputs to CFD model
CFD model validation	IN PROGRESS	Awaiting validation data & LD model inputs
CFD model predictions	FUTURE	Inputs to FEA model
FEA geometry conditioning	IN PROGRESS	
FEA model setup & verification	FUTURE	
Q3 milestone	ON TRACK	ANSYS model setup
FEA model predictions	FUTURE	Insights into materials thermal/stress environment
Q4 milestone	ON TRACK	Combined models benchmarking

LD = low-dimensional (i.e., GT-Power)
CFD = Computational Fluid Dynamics (i.e., CONVERGE CFD)
FEA = Finite Element Analysis (i.e., ANSYS)

Proposed future work

- **Complete combustion modeling** (FY2020)
  - Validate with available data
  - Extend to other speed-load conditions, focusing on more extreme combustion than currently practiced
- **Complete & exercise structural model** (FY2020–21)
  - Focus on spatially varying temperature & stress profiles
  - Provide quantitative guidance for materials research / selection of targets
- **Apply methodology to neutronic engine**
  - Engine currently under design & construction will use neutron techniques to measure stresses *in situ* in an operating engine
  - Will be the first opportunity for comprehensive validation of a combined CFD & FEA approach

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

Responses to prior-year comments

New start — no prior-year review

Collaborations

Model development

- Convergent Science, Inc. helped with initial model setup
- Two OEMs provided design and/or operating data
- Derek Splitter (ORNL/DOE VTO project) provided scan data of LNF head, valves, and piston
- Amit Shyam (ORNL/DOE VTO project) provided light-duty alloy thermophysical data

Validation data

- Scott Sluder (ORNL/DOE VTO project) provided engine data (Co-Optima)
- Derek Splitter (ORNL/DOE VTO project) is providing validation data (PACE)

Results are being shared with multiple PACE/PMCP projects.

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

Collaborations

- Sharing design & materials properties data with engine modeling community

Future work

- Define materials properties needed in future LD engine operation to meet lifespan of needs within constraints

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