Project ID: mat186

Modeling of Light-Duty Engines

Task 4B2 under the Powertrain Materials Core Program (PMCP)

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Bridge to the future for medium- and heavy-duty vehicle propulsion

VTO Powertrain Materials Core Program

3 National Labs, 30+ researchers, 4 Thrust Areas, 17 Tasks

THRUST 1.

Lightweight Alloys (200 – 550 °C)

THRUST 2.

Cost-Effective, Higher Temperature Alloys (550 – 1000 °C)

THRUST 3.

Additive Manufacturing for Advanced Powertrains

TRL 1 — Accelerating Development of Powertrain Alloys — TRL 4

Supported by Adv. Characterization & Computation

THRUST 4.

Atom Probe
Synchrotron
Microscopy
Neutrons
ICME
Thermodynamics
Modern Data Analytics
High Performance Computing

$30M/5 years launched in FY19

Task 4B2 Overview: Modeling of Light-Duty Engines within the Powertrain Materials Core Program

Timeline/Budget

- Task start: October 2019
- Task end: September 2023
- Percent complete: 50%
- **4B2 Budget**
  - **FY20: $125k**
  - **FY21: $125K**

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. Advanced Characterization & Computation

Foundational support for Thrusts 1, 2 & 3
4A. Advanced Characterization / 4B. Advanced Computation

Task	Title	TRL	FY20	FY21
4A1	ORNL Advanced Characterization	Low	$450k	$420k
4A2	Argonne Advanced Characterization	Low	$300k	$300k
4A3	PNNL Advanced Characterization	Low	$300k	$300k
4B1	Advanced Computation	Low	$350k	$400k
4B2	**Modeling of Light-Duty Engines**	**Low**	**$125k**	**$125k**
		Subtotals	$1,525k	$1,545k

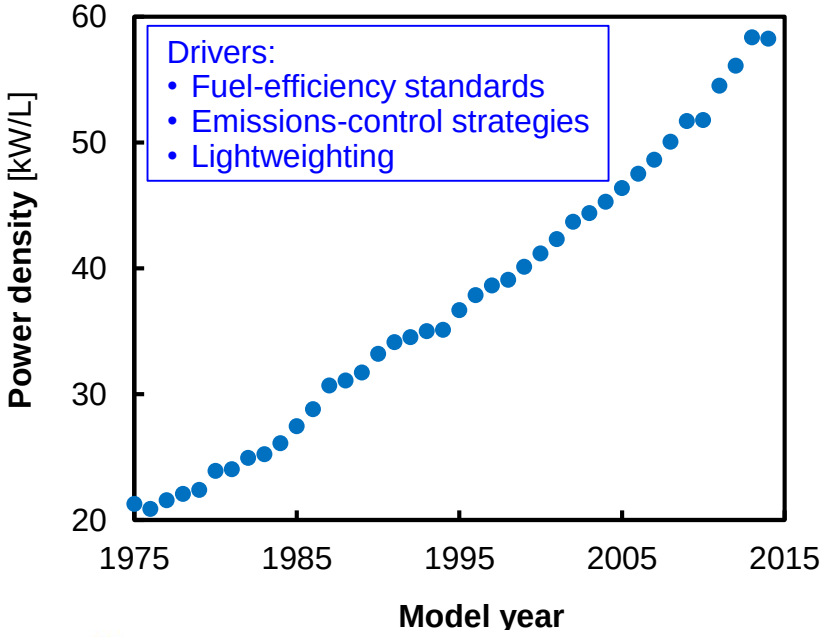
Partners

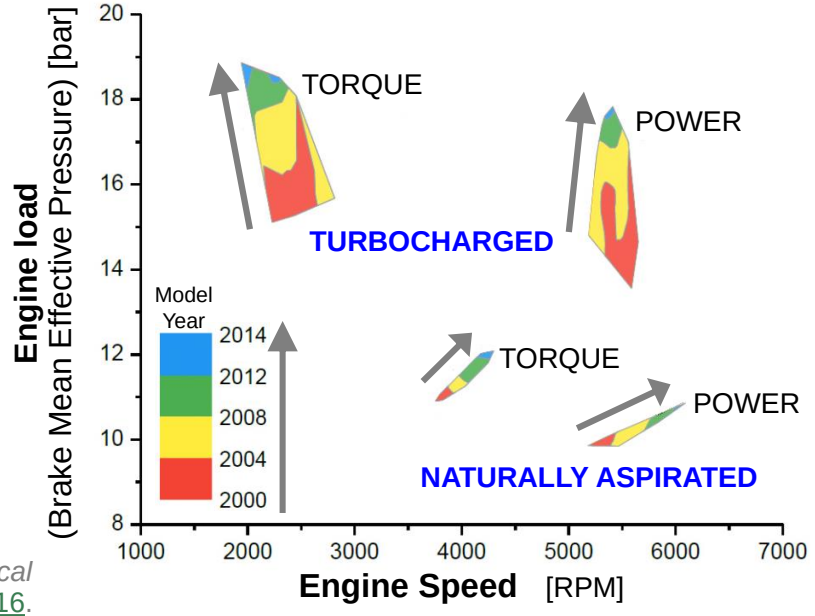
- Task 4B2 Lead
  - Oak Ridge National Laboratory (ORNL)
- Task 4B2 Partners
  - Convergent Science, Inc.
  - Partnership on Advanced Combustion Engines (PACE) & Powertrain Materials Core Program (PMCP) – DOE Vehicle Technologies Office

Materials are limiting future engine development

- **Light-duty engines are increasingly stressed**
  - Causes: **Increased specific output** (power, torque) via downsizing/lightweighting
  - Effects: **Higher pressures & temperatures** → nearing materials temperature limits now
- **New materials can enable higher temperatures**
  - **Reduce protective enrichment** (adding extra fuel to cool components) → increase fuel economy
  - Enable further **downsizing** → increase fuel economy
  - Permit **selective cooling** to optimize engine thermal management & efficiency

Need to understand future operating environment and materials impacts 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.

FY21 Milestones

Date	Status	Milestone
FY21Q2	COMPLETED	Set up and validate low-dimensional & high-dimensional models with advanced heat-transfer and materials thermal solutions for evaluation of engine materials performance
FY21Q4	ON TRACK	Publish study results in the open literature

Project objectives

1 DEFINE FUTURE CONDITIONS

Estimate thermal environment of head, piston, and valves of light-duty and hybrid-electric vehicle engines at increased specific output where current materials will fail.

2 DEFINE MATERIALS PROPERTIES

Estimate required materials properties at component level under projected range of more intensive future operating conditions.

3 LEVERAGE DOE RESEARCH

Integrate with ongoing activities in PMCP* & PACE.**

* Powertrain Materials Core Program, DOE Vehicle Technologies Office

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

4 ADVANCE STATE OF THE ART

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

Materials thermal properties (conductivity, specific heat capacity etc.) for engine-relevant alloys and at high temperatures are generally not published or included in simulations.

This project integrates multiple modeling approaches to evaluate new materials impact on engine efficiency etc

SCOPING STUDY

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

* Eliminate protective enrichment
Explore selective cooling strategies
Enable further downsizing

LDM (Low-dimensional model)
GT-Power

?

How much do specific **new materials** enable improved engine efficiency & where is the most opportunity?

Evaluating new materials developed by VTO under the PMCP

INTEGRATED COMBUSTION AND STRUCTURAL STUDY

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

CFD (Computational Fluid Dynamics)
CONVERGE

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

FEA (Finite Element Analysis)
ANSYS

?

Which materials properties are needed?

Will designs, fuels, etc require new materials?

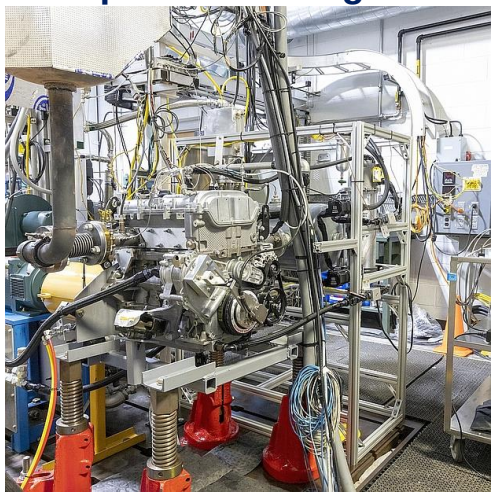
Both studies target modern, production passenger engines run at ORNL & use materials data measured at ORNL.

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

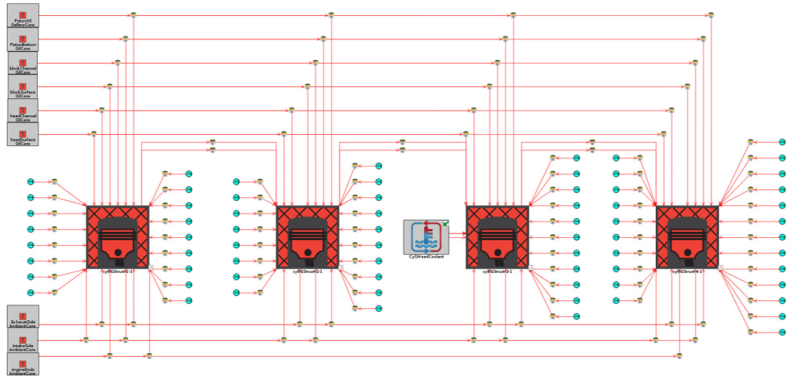
Experimental engine at ORNL

- 2007 GM LNF Ecotec 2L 4-cylinder DISI engine
- Single-cylinder combustion with other 3 cylinders disabled
- Stock OEM piston with 9.2 compression ratio
- Boosted intake
- EPA Tier II fuel
- All validation data at 2000 RPM

◄ Experimental engine



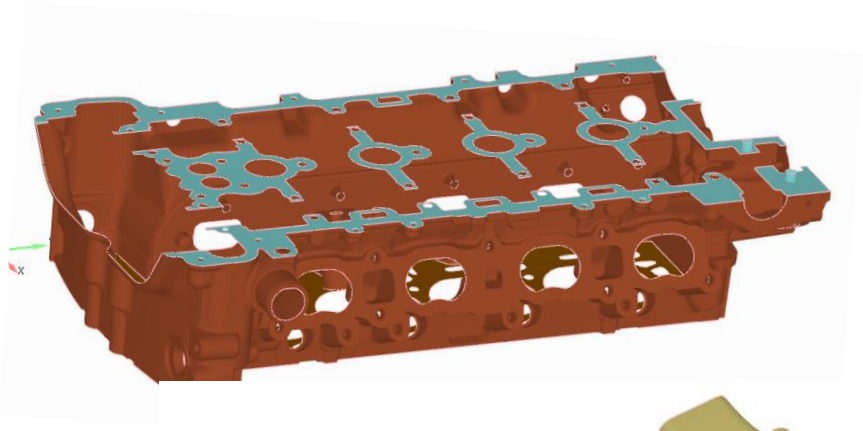
Virtual engine ►

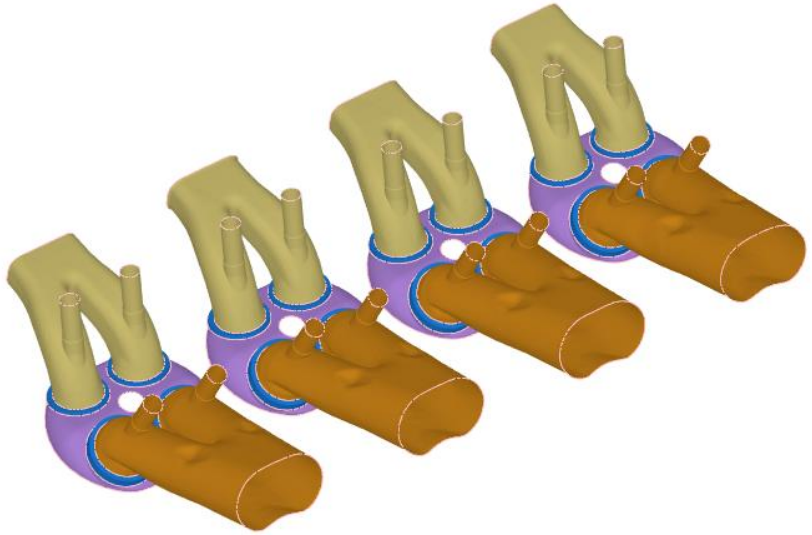


Numerical model

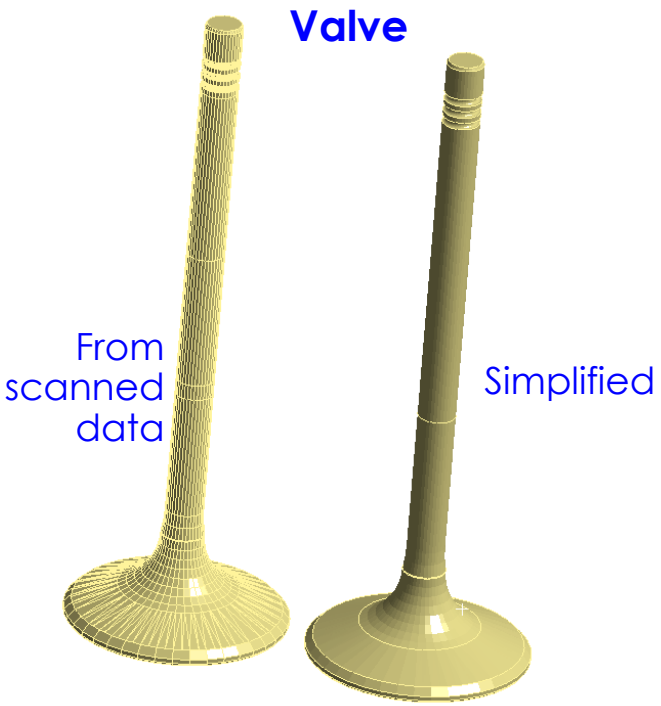
- GT-Power engine model
  - **3-D thermal solver for materials temperatures**
    - **Head discretized into zones with cooling boundaries defined by CFD**
  - **Measured ORNL materials data**
- Combustion & some run data calibrated from experiment
- Study does not account for practical operational factors in achieving load or cooling targets

In FY20, we set up the high-dimensional CFD and FEA models for tuning and study this year





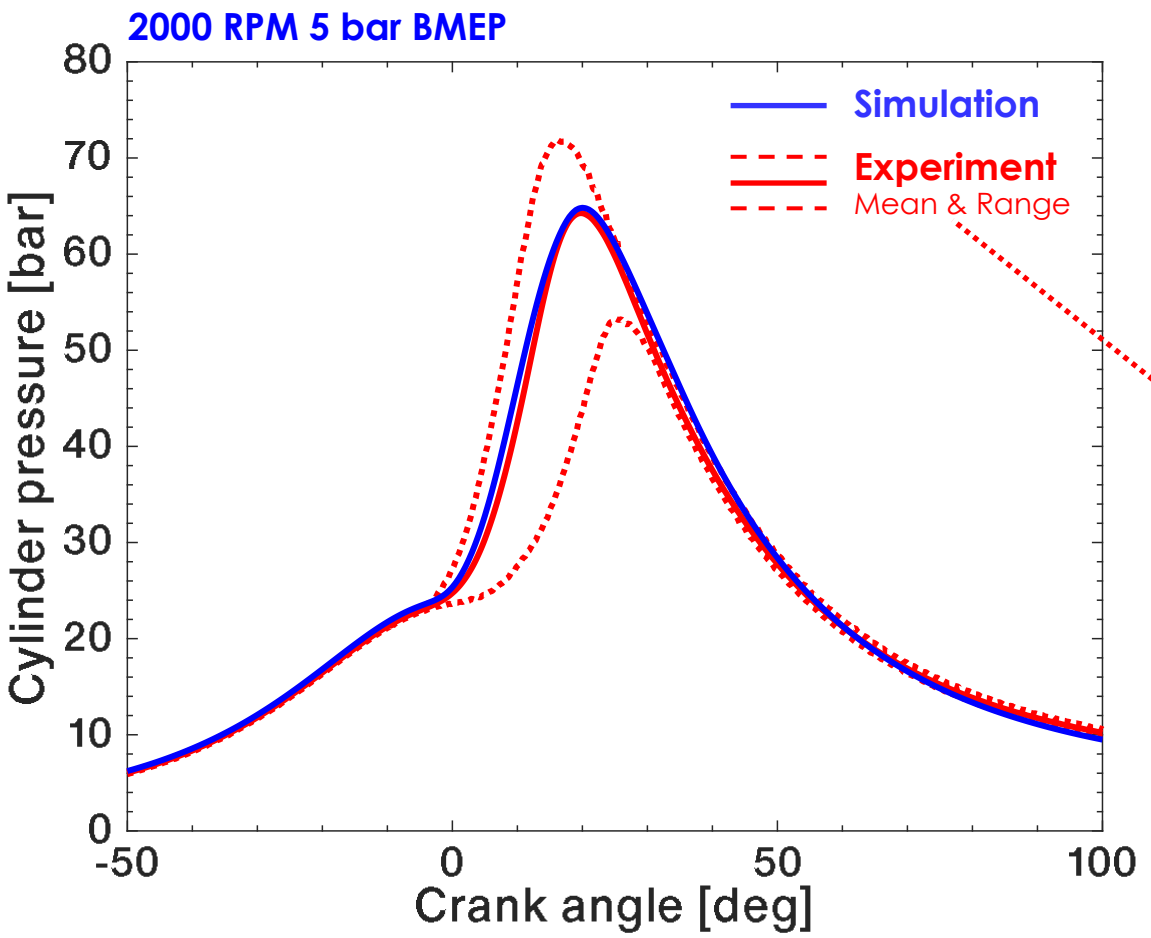
Some of the components imported into CFD model



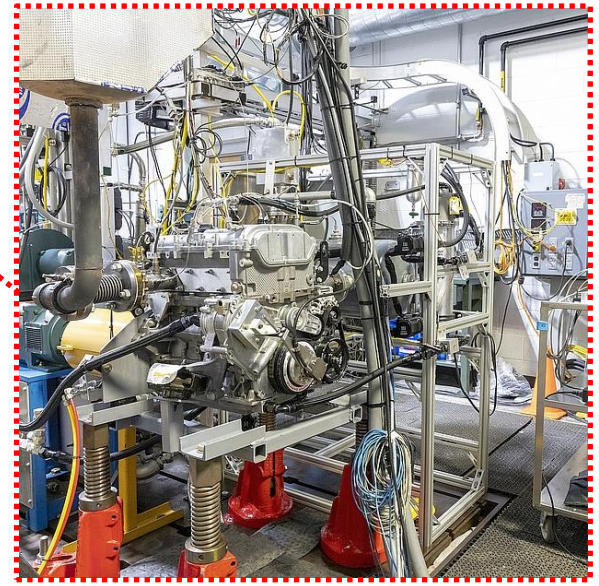
Components conditioned in FEA model

ORNL had physical scans of engine head, piston, and valves which were then imported into the CFD and FEA models. Both models required significant cleanup of surfaces for simplification and run stability.

Both models* were tuned to match experimental data



Cylinder pressure traces, engine power targets, and thermodynamic efficiency were matched within an acceptable experimental variance and uncertainty.



Validated models give confidence in predictions at other conditions.

* LDM and CFD

We compared commercial engine materials for key engine components with a suite of new, higher-temperature alloys being developed under the PMCP for light-, medium- and heavy-duty engines

Engine components	Commercial alloys	VTO-developed alloys	Advantages offered by new VTO alloys	PMCP task
Cylinder head	**A356+0.5Cu** *Cast Al alloy*	**ACMZ*** *Cast AlCuMnZr alloy*	**>50 °C increase vs 356 alloys**, excellent castability, retains strength & stability to >300 °C	1B1 MAT188
Piston	**M126** *Cast AlSi alloy*	**AlCeNiMn*** *3D laser-printed Al alloy*	**>50 °C increase vs cast & forged piston alloys**, retains strength & stability to 400 °C	3A1 MAT189
Exhaust valves	**IN751** *Forged NiCr alloy*	**N21*** *Forged NiFeCr alloy*	**>75 °C increase & lower cost vs IN751**, new class of high strength, polycrystalline alumina-forming alloy capable of >950 °C	2A1 MAT190
Intake valves	**Sil-1** *Forged stainless alloy*	**2079*** *Forged NiFeCr alloy*	**>25 °C increase, higher strength & lower cost than IN751**, higher strength chromia-forming alloy capable of >900 °C	2A1 MAT190
Exhaust manifold	**grey cast iron**	**AFA*** *Cast stainless*	**>100 °C increase**, 10–20× improvement in creep performance, alumina-forming alloy	2B1 MAT184
Block	**319** *Cast Al alloy*	**ACMZ*** *Cast AlCuMnZr alloy*	**>50 °C increase vs 356 alloys**, excellent castability, retains strength & stability to >300 °C	1B1 MAT188

** Alloys developed by ORNL*

Thermal properties of each alloy were obtained or measured as a *f*(Temperature) and provided more accurate input for the virtual engines.

Temperature limit of each alloy was defined by measured or reported tensile properties over a range of higher temperatures.

We focused on materials impacts on higher specific output

Full engine map was explored, but only limited results shown here.

Virtual engine simulation run matrix

- Two speed–load points
  - 2000 RPM 21.9 bar BMEP
  - 5000 RPM 17.7 bar BMEP
- Three power-density load factors
  - 1.00 – baseline engine output
  - 1.25 – 25% increase over baseline
  - 1.50 – 50% increase over baseline
- Three cooling levels
  - Baseline
  - 50% less cooling
  - 50% more cooling

Materials configuration matrix

1. All baseline materials
2. All advanced materials
3. Single-component substitution

Component	Baseline	Advanced
Head	A356+0.5Cu	ACMZ
Piston	M126	AlCeNiMn
Exhaust valves	IN751	N21
Intake valves	Sil-1	2079
Exhaust manifold	Gray cast iron	AFA

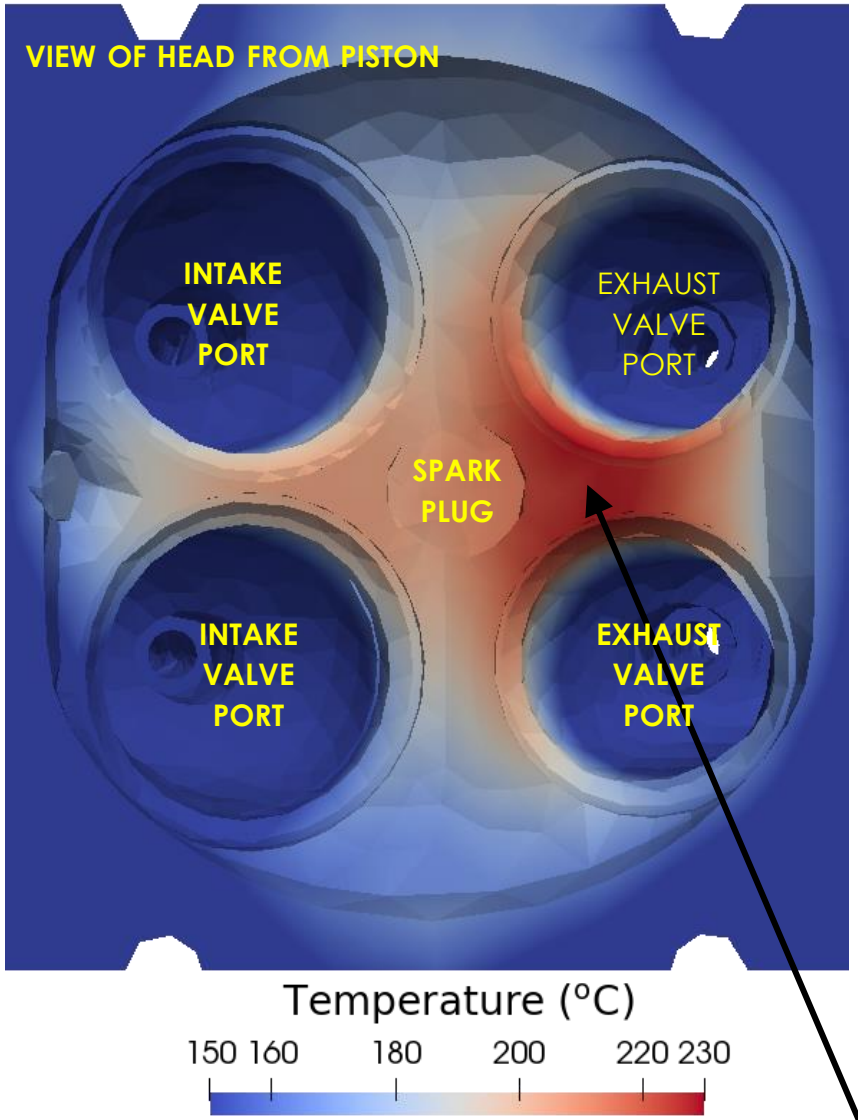
Commercial, production

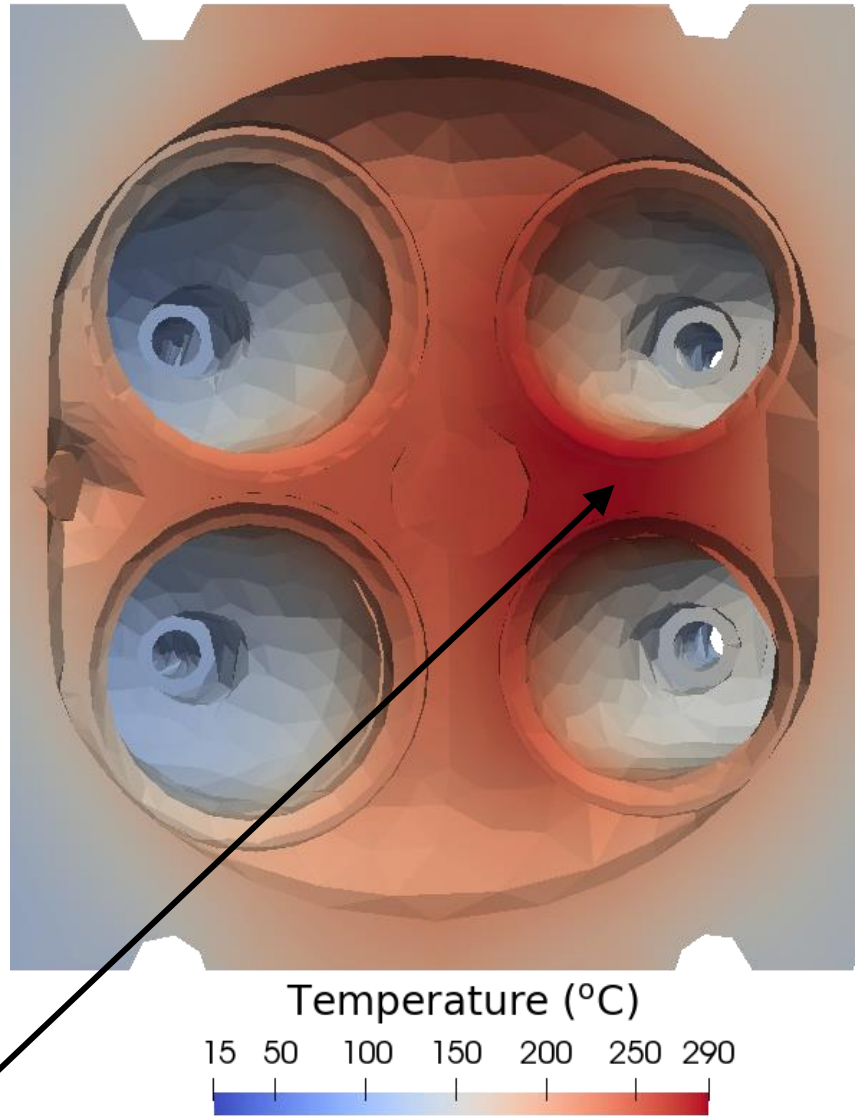
VTO-sponsored ORNL-developed

Targets were component temperatures within materials limits & engine efficiency

Cylinder surfaces have uneven temperature distributions

5000 RPM
Nominal load
Baseline cooling





5000 RPM
1.5× load
+50% cooling

Local hot spots can limit combustion strategy based on materials and lifespan requirements

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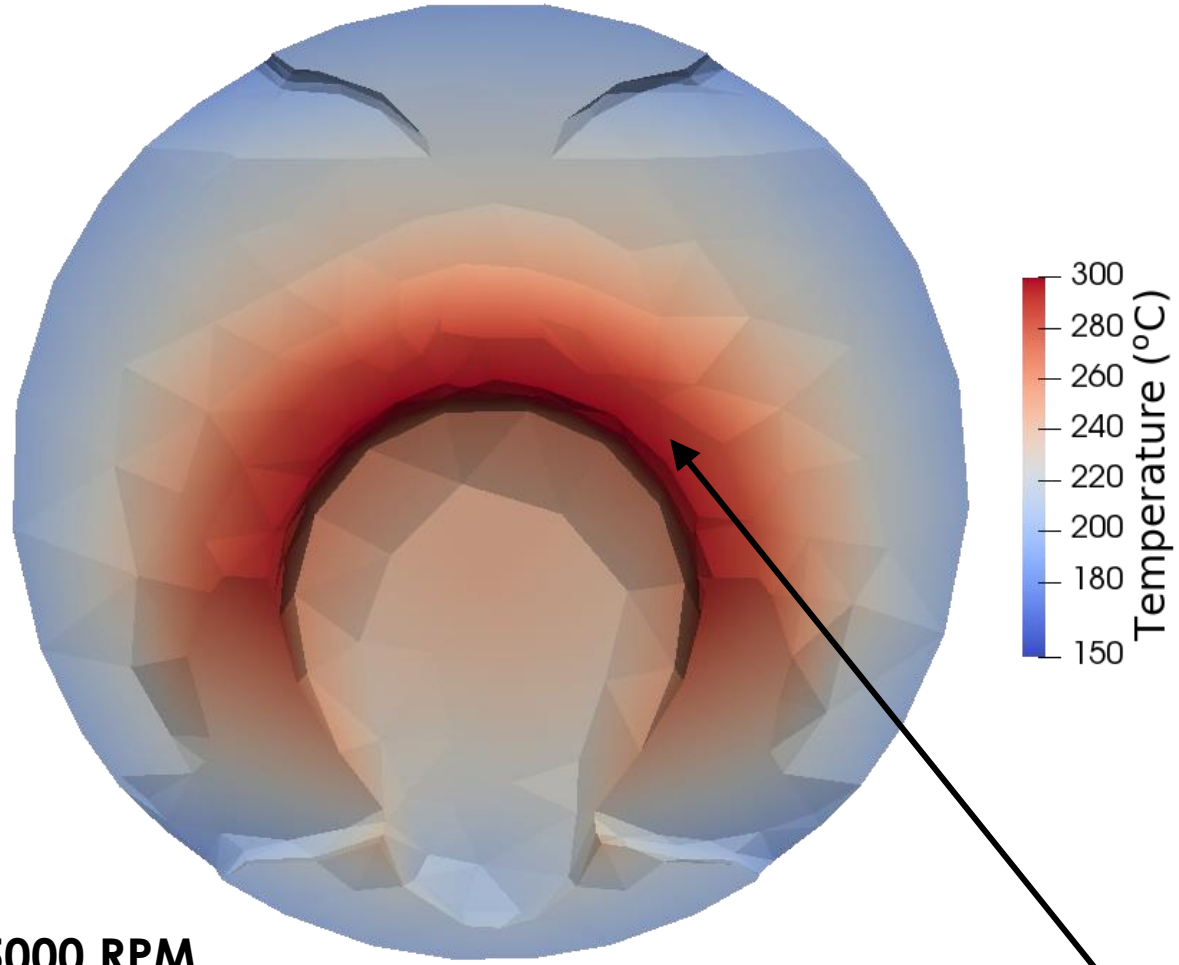
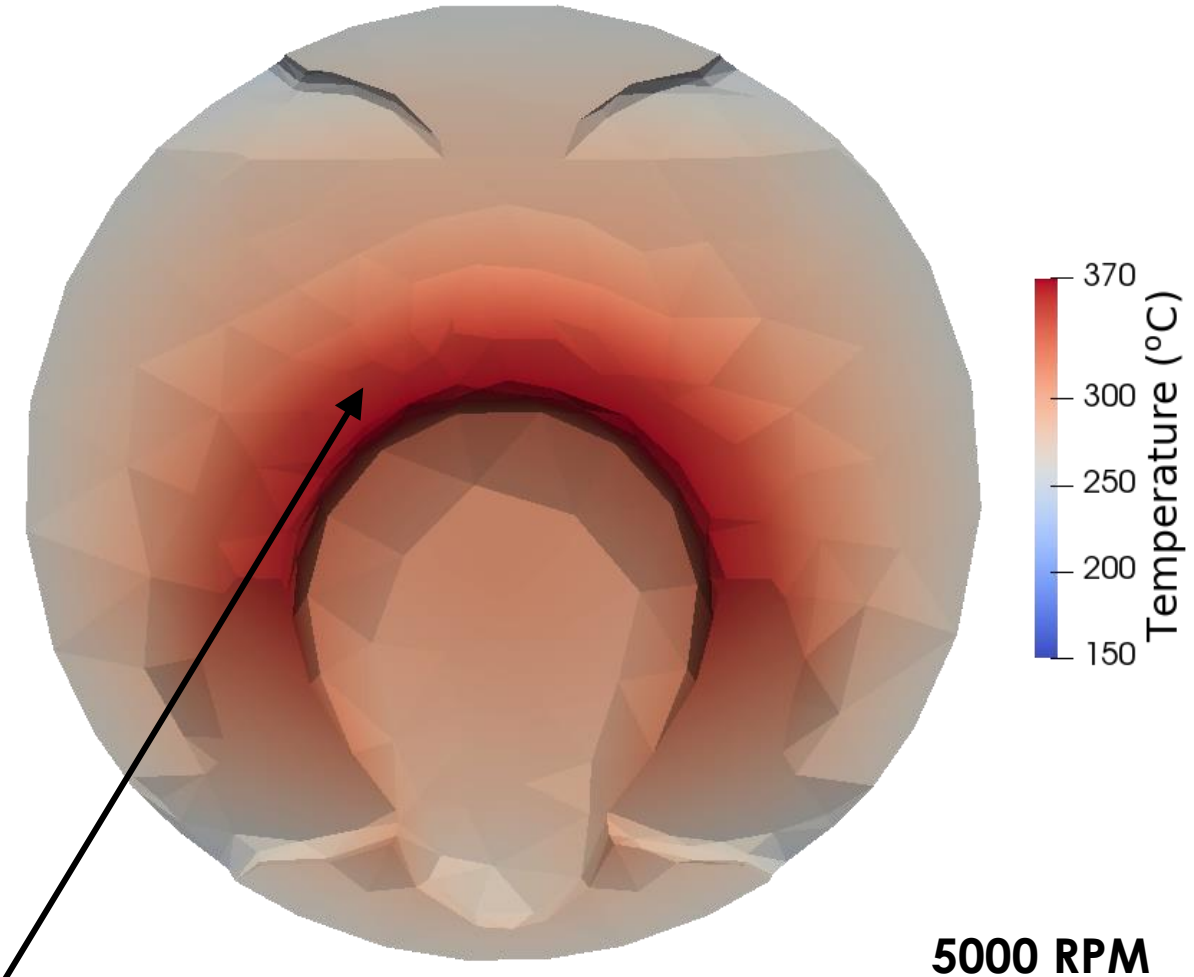
Cylinder surfaces have uneven temperature distributions

VIEW OF PISTON FROM HEAD (PISTON CROWN)





5000 RPM
Nominal load
Baseline cooling

5000 RPM
1.5× load
+50% cooling

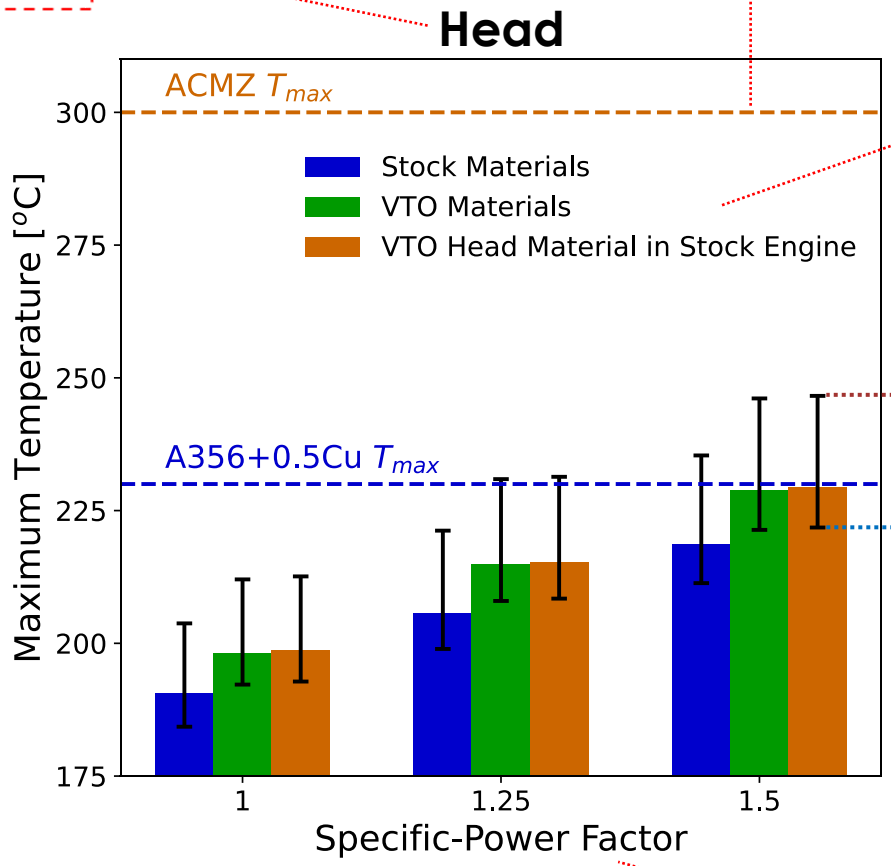
Local hot spots can limit combustion strategy based on materials and lifespan requirements

Increasing specific output raises materials temperatures

2000 RPM

Component of interest

Practical maximum service temperature limit of each alloy



Simulated maximum temperature in component of interest

Materials-substitution scenarios

- Commercial alloys in all components
- VTO-developed alloys in all components
- VTO-developed alloy in labeled component & commercial alloys in all other components

50% LESS

50% MORE

Cooling scenarios

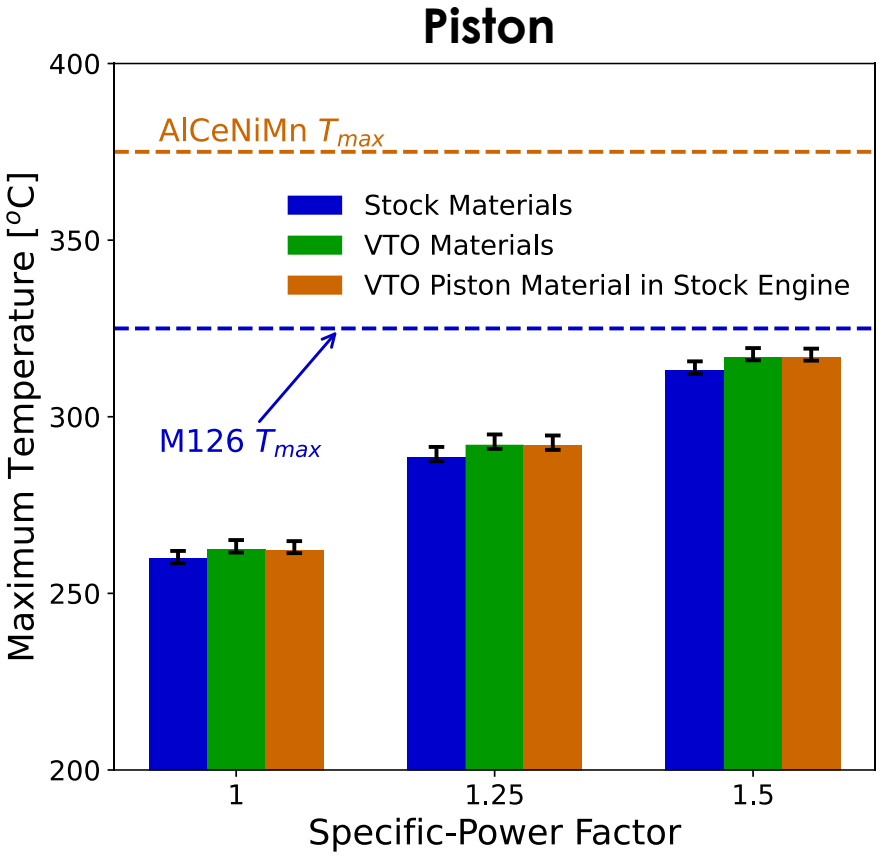
LESS Can less cooling be used (using higher-temperature materials)?

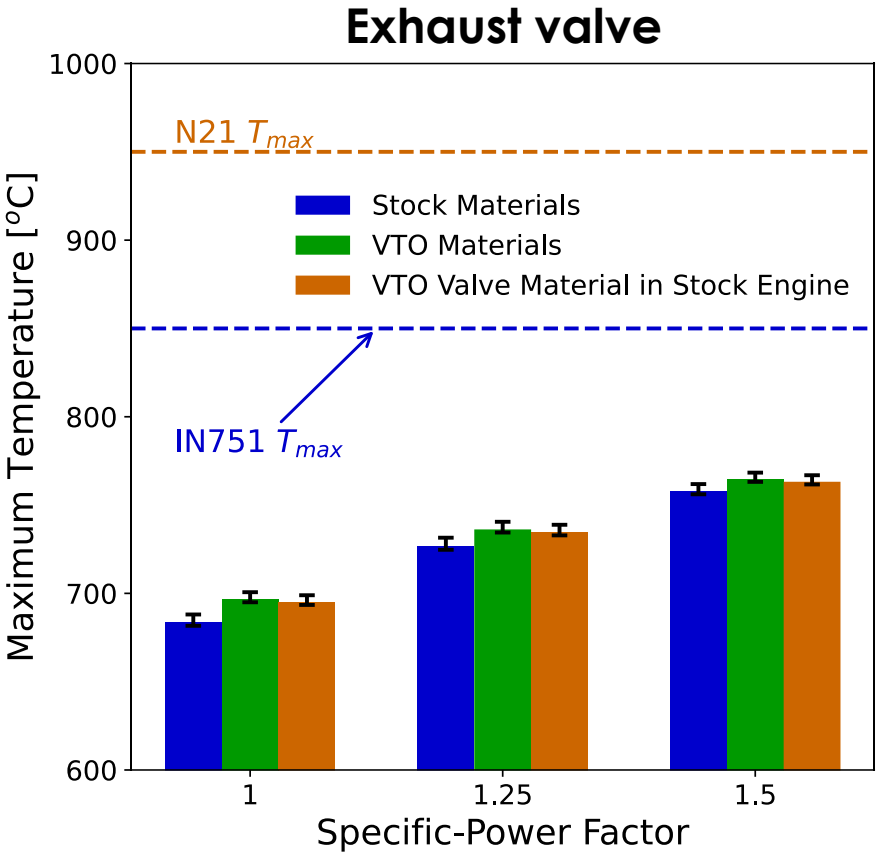
MORE Can more cooling reduce materials temperatures enough?

Target engine brake specific power at baseline and 25% and 50% increases

At 2000 RPM, current materials are sufficient

2000 RPM

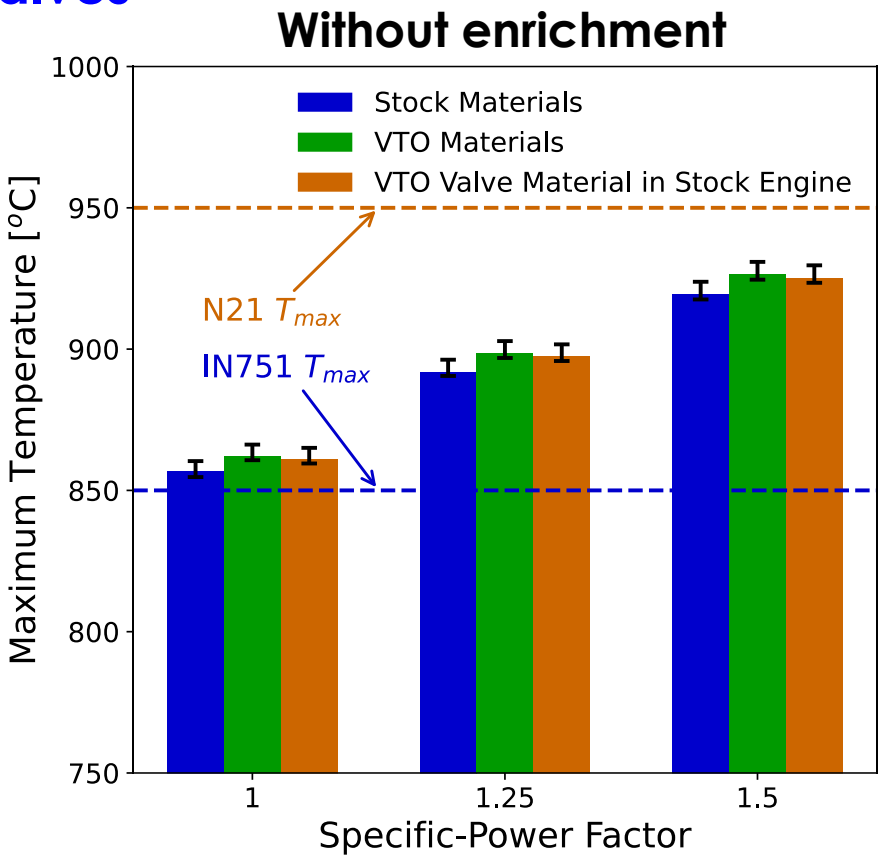


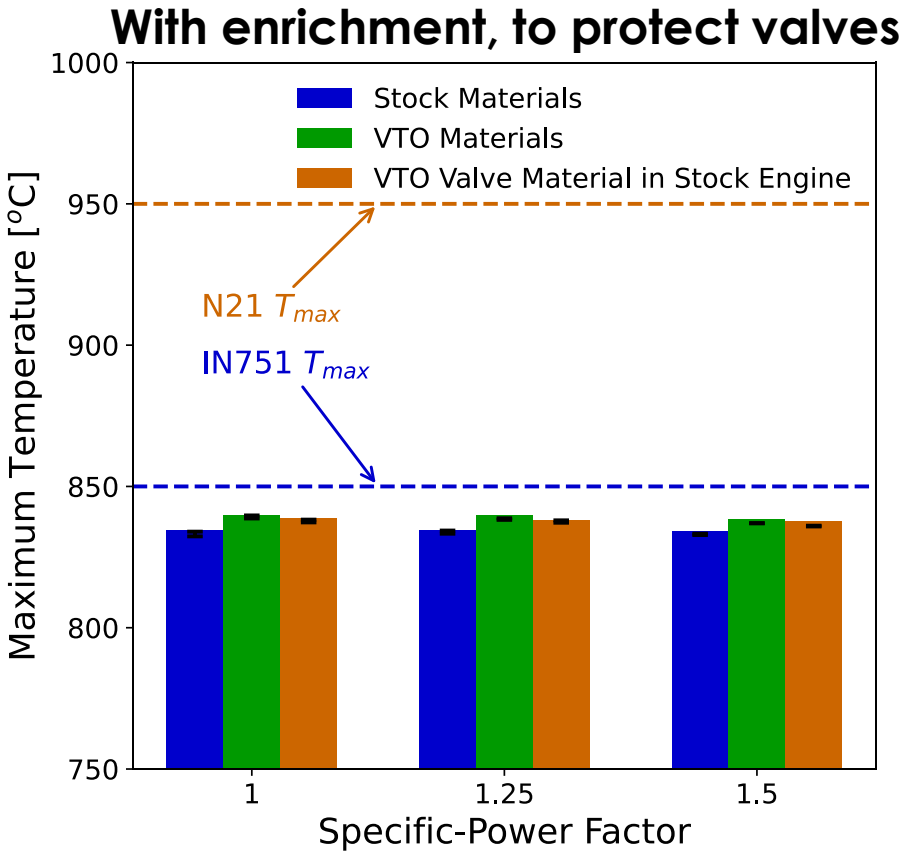


Advanced materials can reduce need for enrichment

5000 RPM

Exhaust valves



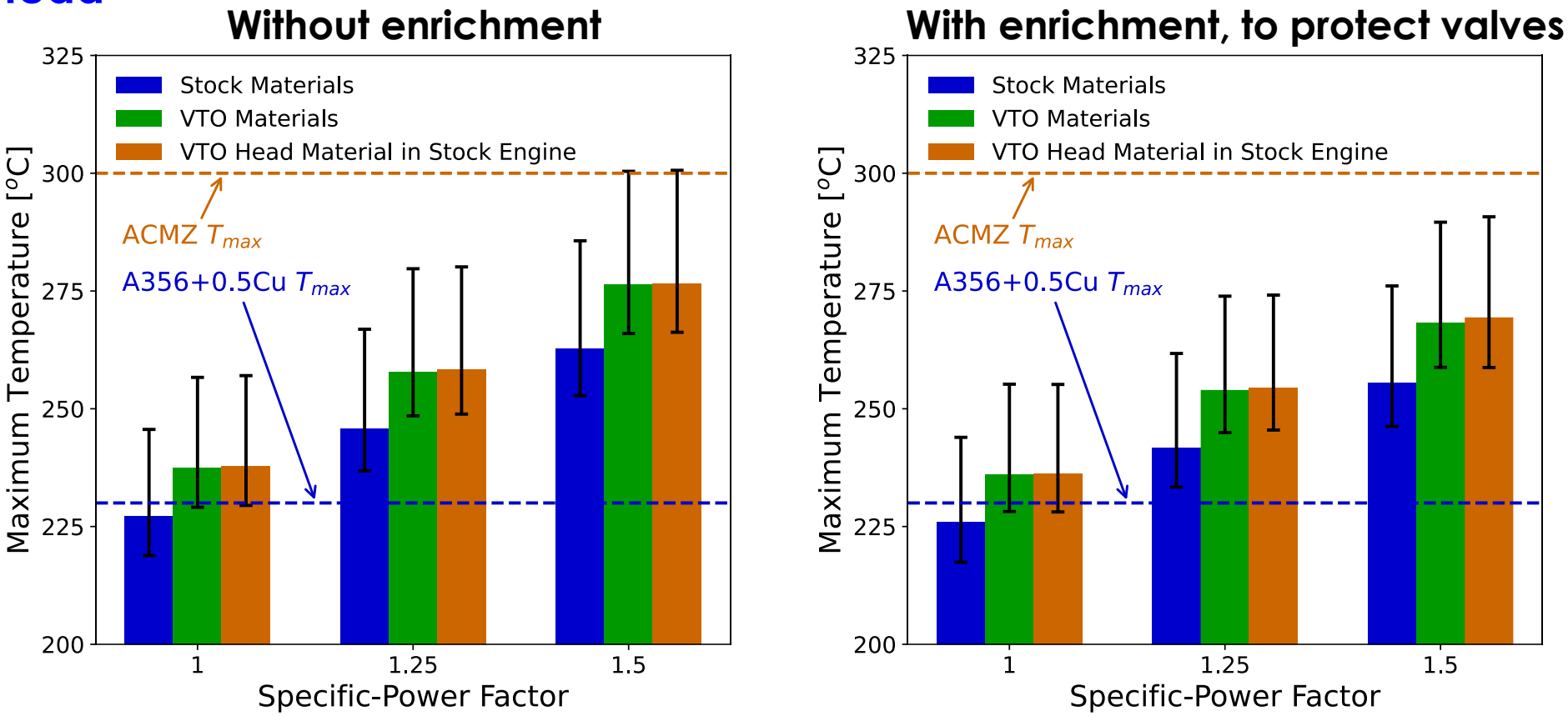


- Advanced materials allow for higher-temperature operation without using extra fuel to cool (enrichment)
- Benefit **~1.5–7% indicated thermal efficiency** (condition-dependent) & better engine-out emissions

Enrichment does not affect cylinder head significantly

5000 RPM

Cylinder Head



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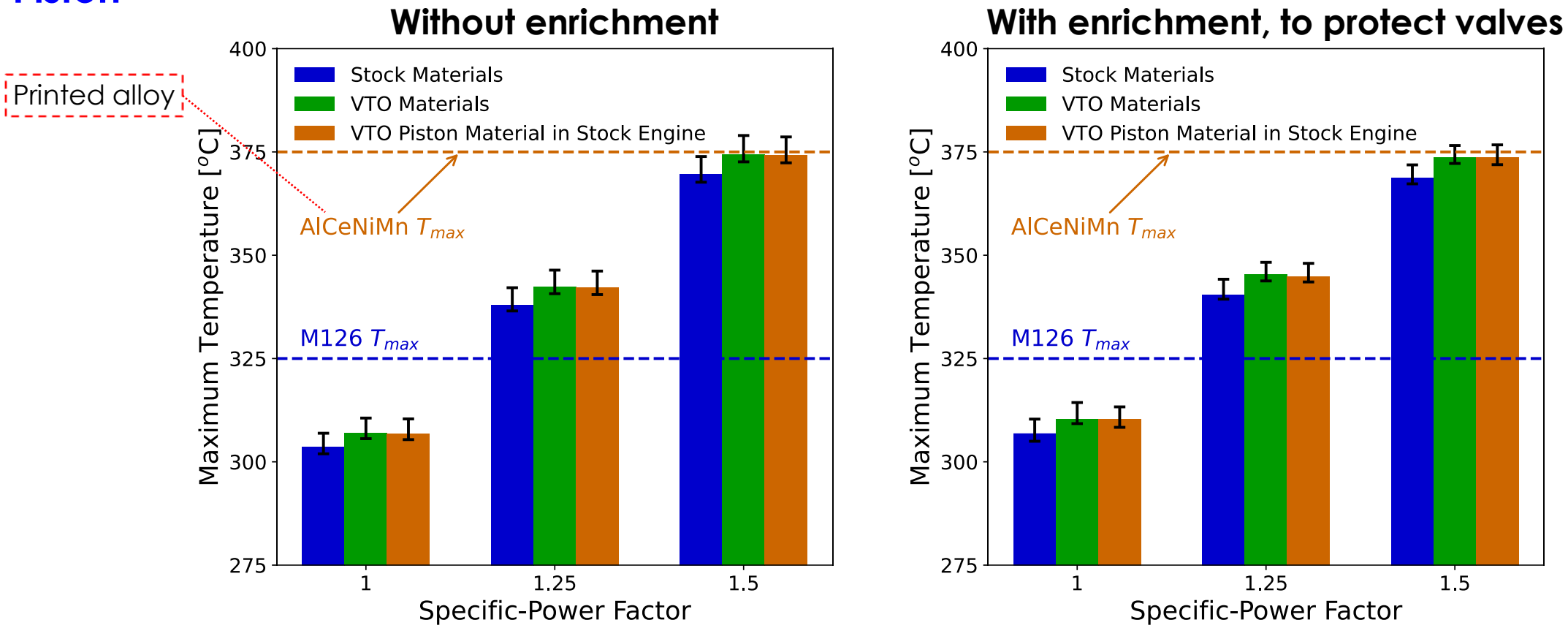
Enrichment does not significantly affect piston

5000 RPM
Piston



- Advanced materials allow for higher-temperature operation without using extra fuel to cool (enrichment)
- Benefit **~1.5–7% indicated thermal efficiency** (condition-dependent) & better engine-out emissions

Implications from modeling

- Increased specific output can increase materials temperatures beyond operating limits of current production alloys

- Advanced, high-temperature materials can …
  - Reduce or eliminate the need for enrichment at high speeds and loads, increasing efficiency & reducing emissions
  - Allow for selective cooling at some operating points, reducing auxiliary loads, and with possible thermodynamic efficiency benefits

- Shifts in combustion heat distribution could lead to increased exhaust enthalpy for waste heat recovery opportunities

Responses to previous-year reviewers' comments

- **Materials properties of interest are not defined (e.g., heavy-duty work with iron will be different from light-duty work with aluminum alloys).**

  This was the first year in a multi-year effort to 1) define the operating environment and then 2) identify which materials properties will be most critical. These properties will vary by component (e.g., creep or oxidation in exhaust valves versus fatigue or wear in pistons versus creep or constrained thermal fatigue resistance in cylinder heads) – these to be determined.

- **This work duplicates work done by OEMs, who have all the design and operating data – who benefits from public knowledge of materials targets?**

  Such information from OEMs is not generally made publicly available to the broader research community. Design of new materials to benefit OEMs leverages 1) more realistic simulations of materials performance at intensified operating regimes and 2) improved state of the art for combustion–materials interface evaluation. OEMs are now testing several of the new target-driven materials developed under the VTO PMCP.

Collaboration and Coordination

- **Project Lead**
  - Oak Ridge National Laboratory (ORNL)
- **Project Partners**
  - PMCP Task 1B1 Properties of Cast Aluminum-Copper-Manganese-Zirconium Alloys
  - PMCP Task 2A1 Oxidation Resistant Valve Alloys
  - PMCP Task 2A2 Higher Temperature Heavy-Duty Piston Alloys
  - PMCP Task 2B1 Development of Cast, Higher Temperature Austenitic Alloys
  - PMCP Task 3A1 Fundamental Development of Aluminum Alloys for Additive Manufacturing
- **Other Collaborations**
  - Convergent Science, Inc.
    - CFD model development & validation
  - Partnership on Advanced Combustion Engines, DOE Vehicle Technologies Office
    - Validation data

Proposed Future Research

- Efforts will include exploration of the full operating map to identify opportunities from advanced materials
- Refine results with high-fidelity model (CFD)
- Apply concepts to enable peak-efficiency engines for hybrid electric vehicles and range extenders
- Apply concepts to medium- and heavy-duty vehicles

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

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

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 light-duty and hybrid electric vehicle operation to meet lifespan of needs within constraints