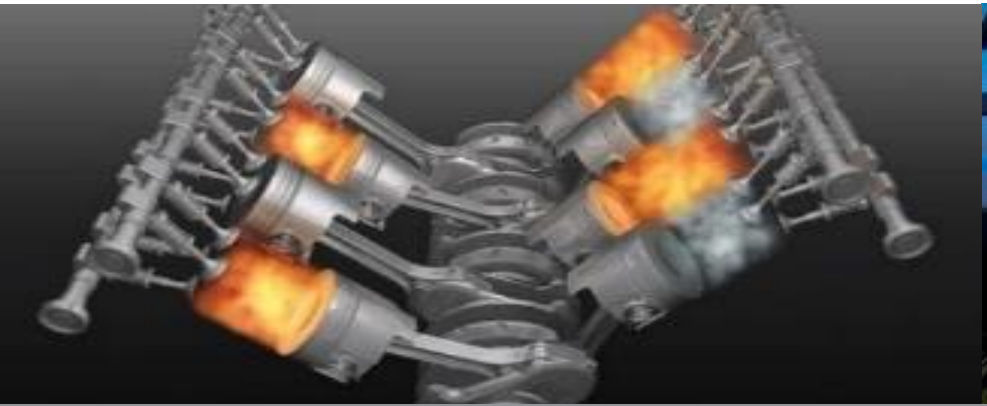
PARTNERSHIP
TO ADVANCE
COMBUSTION
ENGINES

Partnership for Advanced Combustion Engines (PACE)
– A Light-Duty National Laboratory Combustion Consortium

Isaac Ekoto, Matthew McNenly (presenter), Paul Miles, Sibendu Som, Jim Szybist

VTO Annual Merit Review
June 22, 2021, 10:00 am EDT
Project ACE138



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Overview

Timeline

5-year program

- Start Date: FY19 Q3
- End date: FY23 Q4
- Percent complete: ~46%

US fiscal years run from October 1 through September 30

Barriers and Technical Targets*

- Development of enhanced understanding and predictive models to address:
  - Limits to SI engine efficiency (knock/LSPI)
  - Barriers to highly dilute combustion
  - Emissions reduction (cold start)

* Aligned with USDRIVE ACEC Tech Team Priority 1: Dilute gasoline comb.

Budget

- Total PACE FY21 budget $8,920K
- Approximate allocations
  - Knock/LSPI mitigation ~ 30%
  - Dilute combustion ~ 30%
  - Emissions reduction ~ 40%

Budget breakdown by task provided in reviewer only slides

Partners

- ANL, LLNL, NREL, ORNL, SNL
- USDRIVE ACEC Tech Team

Project leads

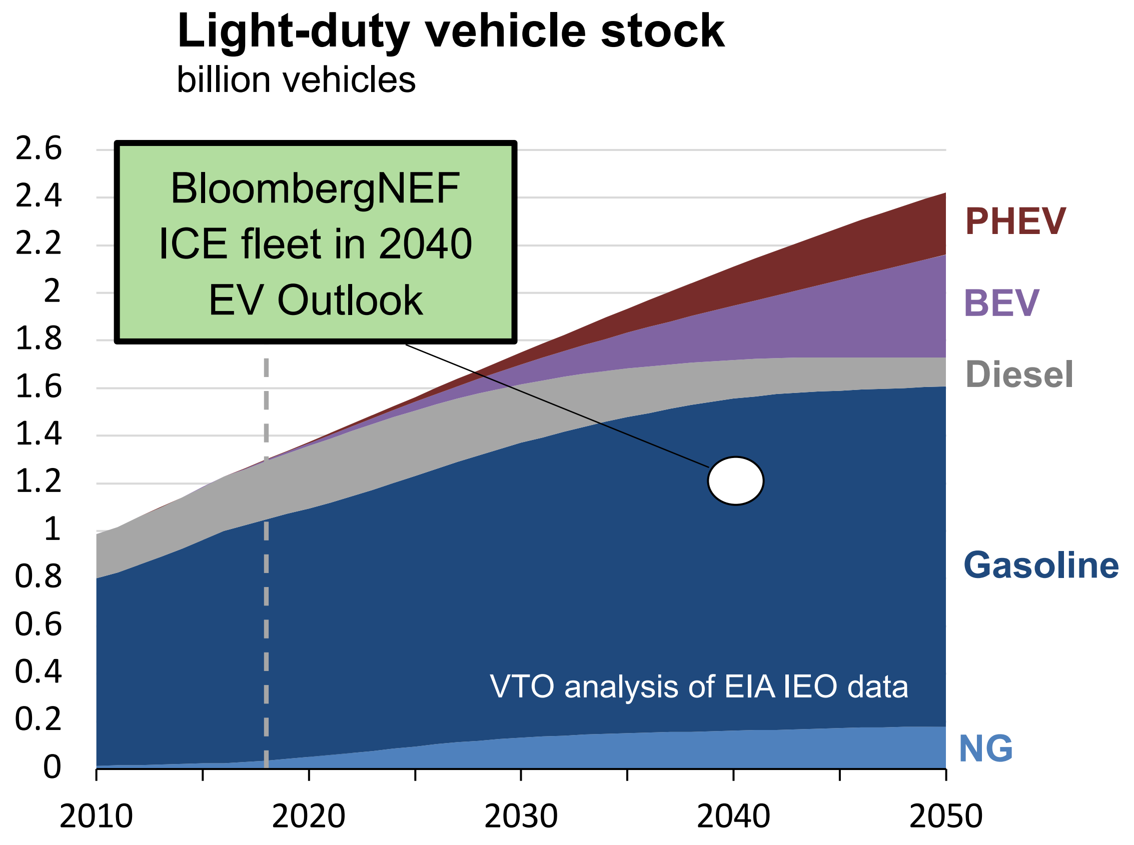
- I. Ekoto (SNL)
- M. McNenly (LLNL)
- S. Som (ANL)
- J. Szybist (ORNL)

Relevance | Improved ICEs are key to energy and environmental security

Approximately 400 million light-duty vehicles with ICEs will be sold in the US between now and 2050 (2.4 billion worldwide)

- Improving ICE efficiency is a critical element of a path toward lower petroleum consumption and greenhouse gas emissions
- Tailpipe pollutant emissions can be reduced to near zero – alleviating urban environmental concerns
- US competitiveness secures over 900K manufacturing jobs (Mar. 2021 - U.S. Bureau of Labor Statistics)

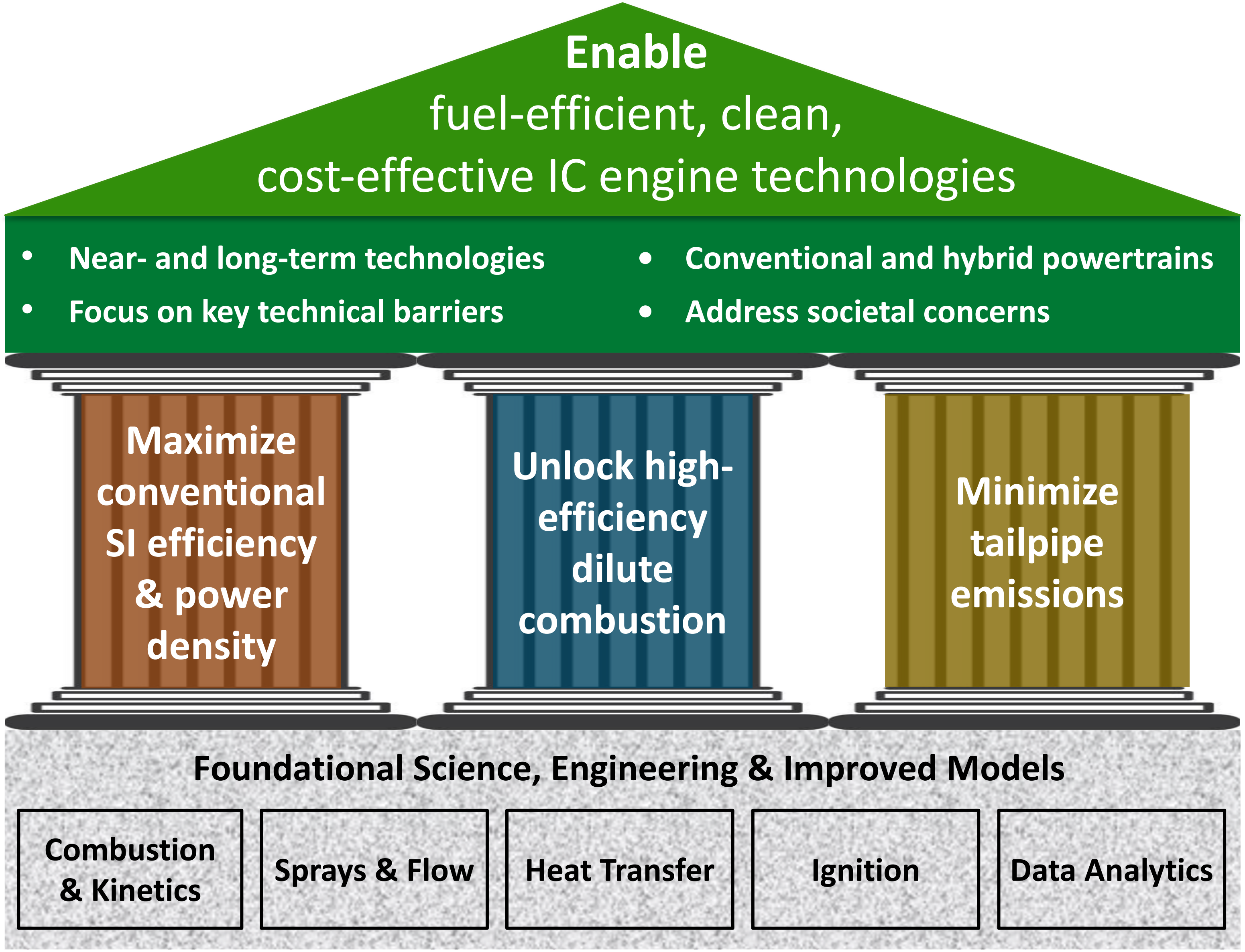
2019 International Energy Outlook, EIA



Relevance | Improved ICEs are key to energy and environmental security

Our end-goal will be reached through progress in three key areas:

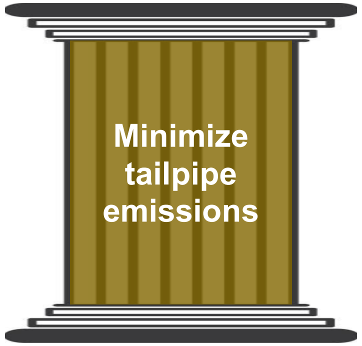
- Knock and LSPI mitigation for stoichiometric SI engines
- Improving stability & efficiency of highly dilute combustion
- Reducing emissions to a zero-impact level (focus on cold-start)



Relevance | Improved ICEs are key to energy and environmental security

- **Improved knock and LSPI control**
  - Near-term benefit with potential for > 5% efficiency improvement

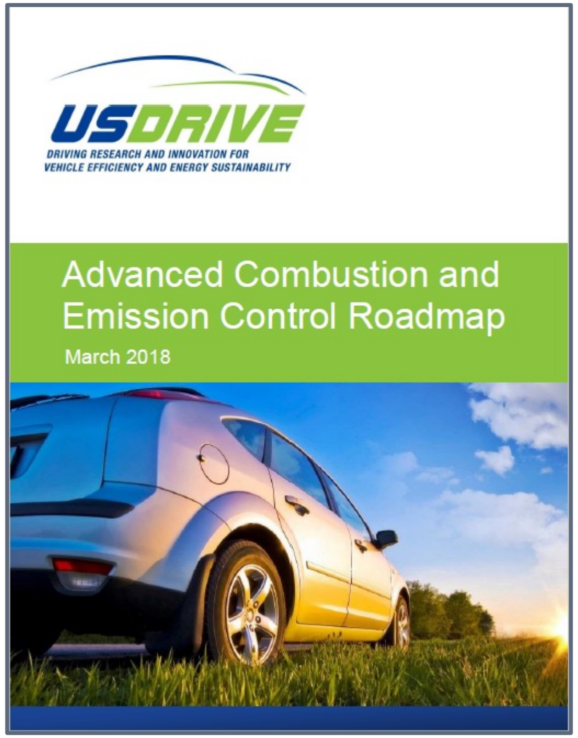
- **Highest potential efficiency gains but significant barriers**
  - Mid-term, high EGR stoichiometric for > 12% efficiency gain



- **Deeper understanding of cold start physics and chemistry enables numerically-aided design and calibration**
  - Tier 3 Bin 20 emissions levels and beyond

Approach | Research is aligned with industry priorities and workflows

- Strong alignment with USDRIVE ACEC Tech Team
- *Ab initio* engagement on plans and success measures



PACE

Open source models

ANSYS

CONVERGE

GT POWER

SIEMENS

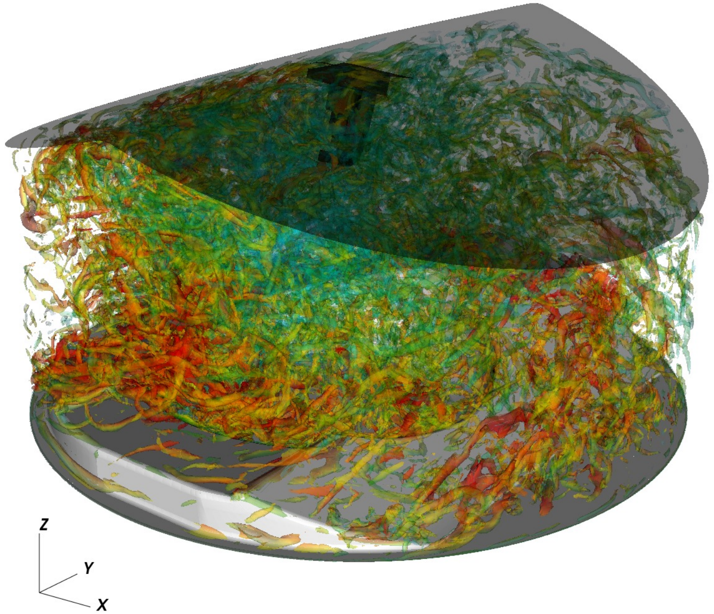
Everyone Welcome

- Direct path toward impacting OEM workflows
  - Software vendors integrated into AEC MOU meetings
  - OEM user-ready submodels as task deliverables – explicit UDF examples

Approach | Leverages DOE investment in HPC and ML/AI

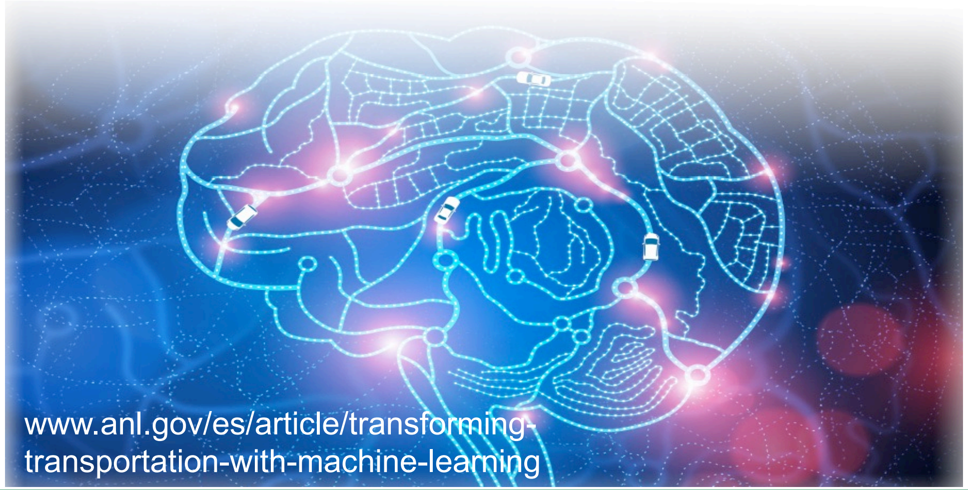
- HPC will be used as a microscope – illuminating processes that are inaccessible to experimentation

- HPC simulations provide a benchmark for accuracy of engineering simulations



Source: ANL

- Machine learning and pattern recognition will be applied to
  - Resolve decades-old problems (*e.g.* root causes of cyclic variability)
  - Detect and mitigate abnormal combustion (instability, knock, LSPI, misfire)
  - Develop expert systems enabling optimal CFD-based design
  - Develop data-driven efficient sub-models



Improved knock and LSPI control

Major Outcome 1: Models for combustion system analysis accurately predict knock response to design changes

Success measure: *Simulation of changes in engine geometry or operating conditions predicts the change in KLSA within 1 degree over the knock limited operating range of the engine, with a 5X reduction in simulation time.*

Major Outcome 2: Data analytics enable operation and real-time control to mitigate knock/LSPI

Success measure: *least 10 CAD before knock occur*

Similar machine learning tasks for Dilute and Cold Start pillars leading to GO/NO-GO for FY23 engine validation

Major Outcome 3: Develop new multi-step phenomenological mechanism for LSPI that captures wall-wetting, lubricant, and geometry effects

Success measure: *Phenomenological model captures relevant physical causes of preignition and demonstrates pathways to reduce the occurrence of LSPI by 50%.*

Major Outcome 4: Improved high-load igniter performance and igniter durability enabled by predictive modeling

Success measure: *An ignition model including spark-plug geometry and electrical discharge circuit details predicts spark stretch, blowouts and restrikes, and flame initiation, propagation and quenching. The model can accurately predict 0-5% mass burned fraction within 10% (mean and standard deviation).*

Approach | All tasks support 7 Major Outcomes

High-efficiency, low-variability dilute combustion systems

Major Outcome 5: Major Outcome 5: Homogeneous and stratified lean/dilute engine efficiency and emissions are accurately predicted

Success measure: *Validated simulations predict the change in burn duration and COV (to within 10%) relative to a baseline configuration for a change in engine design at 30% dilution and ACEC 3 bar/1300 rpm test point.*

Major Outcome 6: Develop viable advanced igniters and control methods that expand existing dilution limits and enable stable catalyst heating operation

Success measure: *Prototype igniters and control strategies ignition control methods enable stable ignition for EGR dilution rates of up to 40% or air dilution rates of up to 50% with no adverse impact on pollutant emissions relative to the stock OEM configuration. Demonstrate ignition system can maintain stable combustion at high exhaust heat flux conditions seen during cold start. ACEC 3 bar/1300 rpm test point.*

Major Outcome 7: … pression ignition combustion …

Success measure: *Co … 100 N-m-s^{-1} and a pathway identifi … erating points*

PACE sharpens research focus on tasks with greatest relevance to the light-duty OEMs

Approach | All tasks support 7 Major Outcomes

Cold-start design and calibration capability

Major Outcome 8: Validated cold start modeling capability that accurately predicts injection and spark timing trends on:

- Cold-start engine-out emissions
- Combustion phasing and stability
- Exhaust heat losses and oxidation (accurate catalyst feed-gas enthalpy and composition)

Success measures:

- > 80% accuracy in predicting engine-out emissions and stability for nominal conditions (relative error in emission level < 20%)
- ACEC cold start protocol COV must be less than 20% (> 80% accuracy)
- > 80% accuracy predicting feed-gas emissions and stability for operating conditions matched to PACE cold-start experimental data set
- > 90% accuracy in predicting heat losses in hot end exhaust for varying heat flux conditions

Accomplishment | PACE team made significant progress during the pandemic

Severe Acute Respiratory Syndrome coronavirus 2 (SARS-CoV-2)

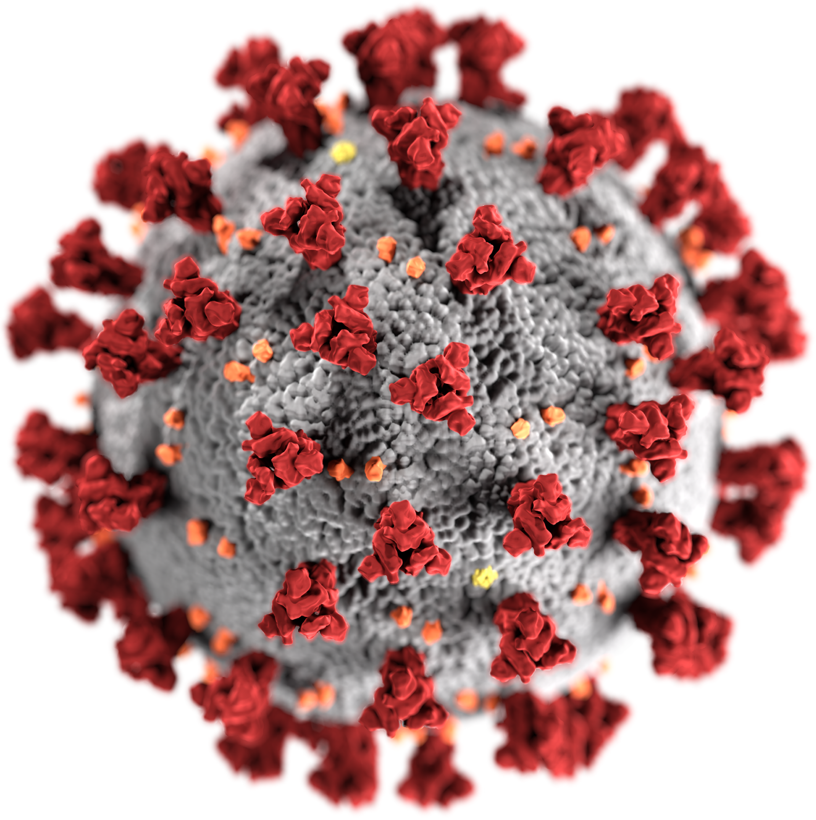


Photo Credit: A. Eckert, MSMI, D. Higgins, MAMS

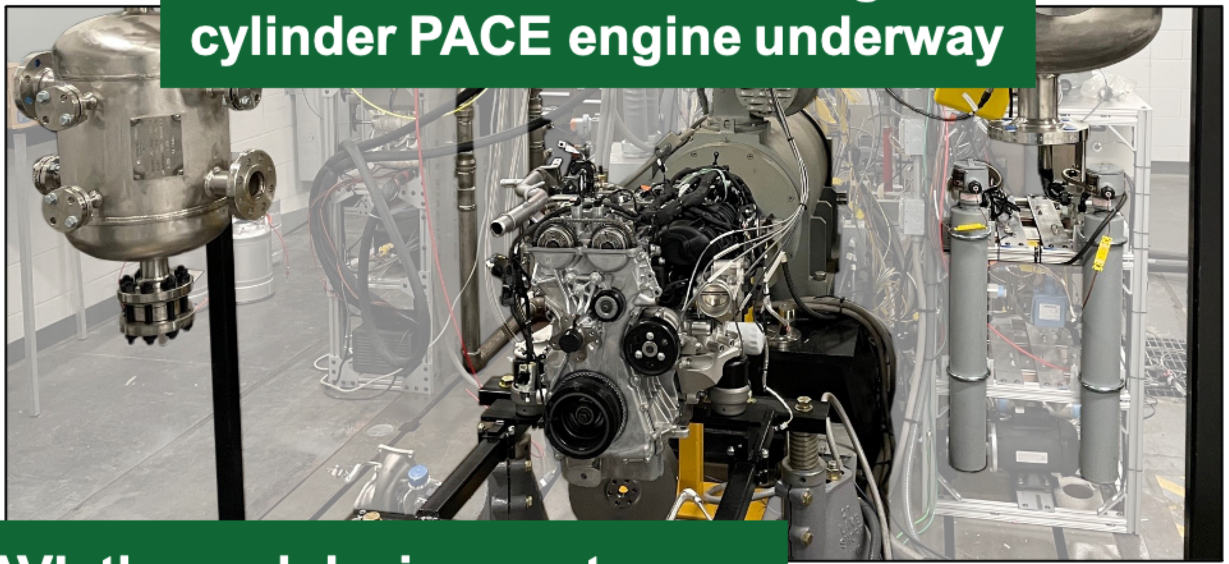
- All national labs shutdown March 2020, except ORNL
- Supercomputing resources diverted to emergency COVID-19 projects.
- Experimental facilities started returning to service Summer 2020 (except ANL APS and ORNL SNS).
- Simulation and theory teams at ANL, LLNL, NREL, ORNL, and SNL are still remotely working.
- Most milestones were delivered on time, while nearly all those that were late were delayed only 3 months (or less).

True testament of the ingenuity and team spirit of the PIs to adapt to the new reality, reprioritize tasks, and continue steady progress on the PACE objectives

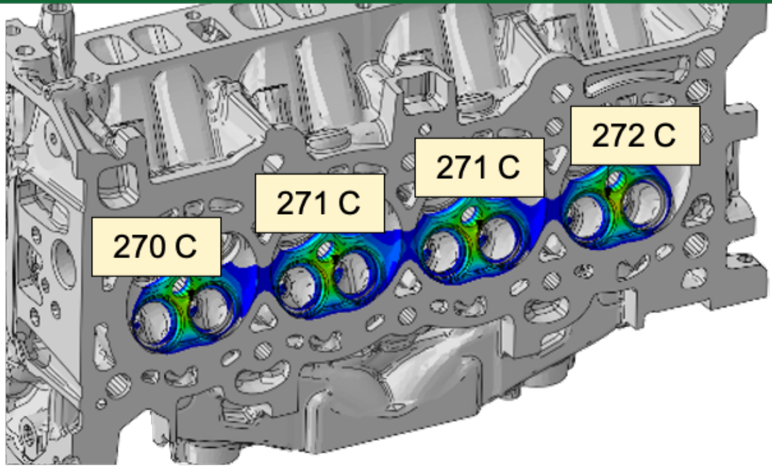
Accomplishment | PACE 2.3L common platform engine purchase complete

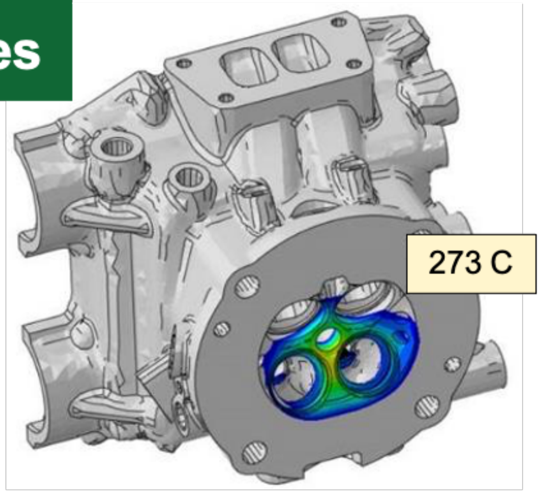
- PACE engine contract awarded to AVL Sept. 2020 for two engines
- Common platform designed to match a production 2.3L turbocharged engine as closely as possible
  - ANL - metal single-cylinder engine
  - SNL - optical single-cylinder engine
- AVL delivery on-track for Nov. 2021
- ORNL to install two similar engines
  - single cylinder with multi-cylinder block (on-track for Q3FY21)
  - multi-cylinder for cold-start tests

Installation of ORNL single-cylinder PACE engine underway



AVL thermal design captures multi-cylinder wall temperatures





Accomplishment | Consensus achieved for PACE-20 as the common surrogate

metric	RD5-87(#2A)	PACE-1	PACE-20	EPA Tier III
RON [1]	92.3	91.8	92.1	92.3
MON [1]	84.6	82.3	84.5	84.5
H:C [1]	1.98	1.97	1.97	1.96
density [g/mL] [1]	0.75	0.75	0.74	0.75
PMI [2]	1.68	1.56	1.50	
	D86	D86	D86	D86
T_{10} [C] [1]	57.8	60.4	57.9	52.7
T_{50} [C] [1]	101.3	100.6	89.9	91.2
T_{90} [C] [1]	157.9	165.8	166.0	159.5

[1] Measurements from SWRI and Gage (ASTM D2699, D2700, D5291, D4052, D86)

[2] Calculated from DHA (ASTM D6729)

- Extensive validation completed since AMR20:
  - low and intermediate heat release in engine and RCM (ace139 – Wagnon)
  - free spray plumes (ace143 – Powell)
  - spray wall interaction (ace144 – Pickett)
  - spray collapse in engines (ace167 – Torelli)
  - soot volume fraction (ace168 – Manin)
  - soot pyrolysis (ace168 – Manin)
  - flame speed (ace139 – Wagnon)
  - improved chemistry (ace139 – Wagnon)
- 15 barrels (54 gal.) ordered from Gage
- 7 barrels of PACE-20 BOB also ordered

Accomplishment | Discontinued FY20 project to bolster investment in 4 areas

Focused PACE on two DOE Exascale Computing Program codes leveraging $18M ASCR investment in NEK5000 ($8M) and Pele ($10M)

Dedicated CFD integration tasks for Major Outcomes 1 and 5 to quantify new models:
- spray-wall
- ignition
- turbulent-chemistry
- conj. heat transfer
- spray nozzle
- flame quenching
- emissions
- algorithmic speedup

Securing common set high-pressure injectors
- 25 Bosch Motor Sports injectors (500 bar)
- complete laser light sheet patternation data
- best match will be the primary set with the rest serving as spares for the program

Increased Spray Simulation Task Support
- full accuracy test
- spray w/cross flow
- 17 free spray conds.
- vaporization in VOF
- near-field plume corrections
- non-flashing vaporization
- discrete particle to Eulerian for wall films

Built new optimization tools for accurate and smaller reduced mechanisms
- Eliminates main human-in-the-loop iteration
- Easily optimize over 80 reactions (simult.)
- 10^8 ignition calculations used in a month to reduce PACE-20 model to 315 species

Accomplishment | 1 month with new tools is set to save an expected 25% in CFD costs

Improved detailed kinetic model after validating against 5,500+ ignition delay times and 1,100+ laminar flame speeds including PACE-20 neat components and their mixtures. See ace139 (Wagnon).

Detailed kinetic model
4,000+ species

Global Pathway Selection [1]

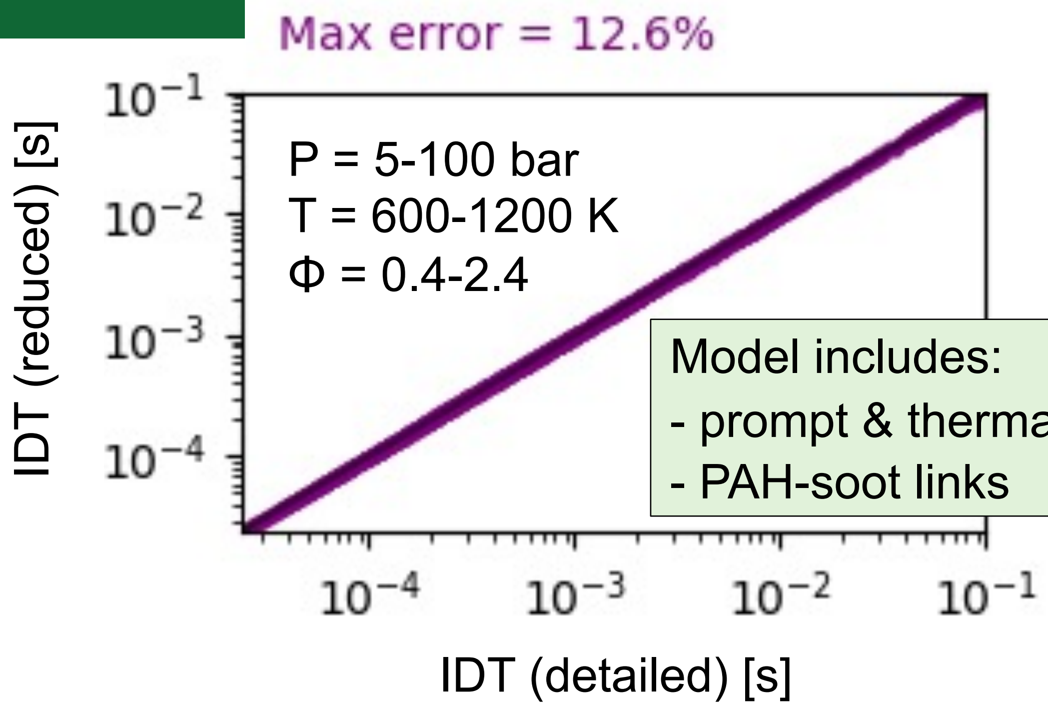
Zero-RK

Isomer identification and lumping

See ace140 (Whitesides)

Reaction rate constant optimization

A 315 species reduced kinetic model for PACE-20



Model includes:
- prompt & thermal NOx
- PAH-soot links

Impact: A robust, accurate, and computationally cheaper kinetic model is available for use in engine simulations. See ace145 (Edwards)

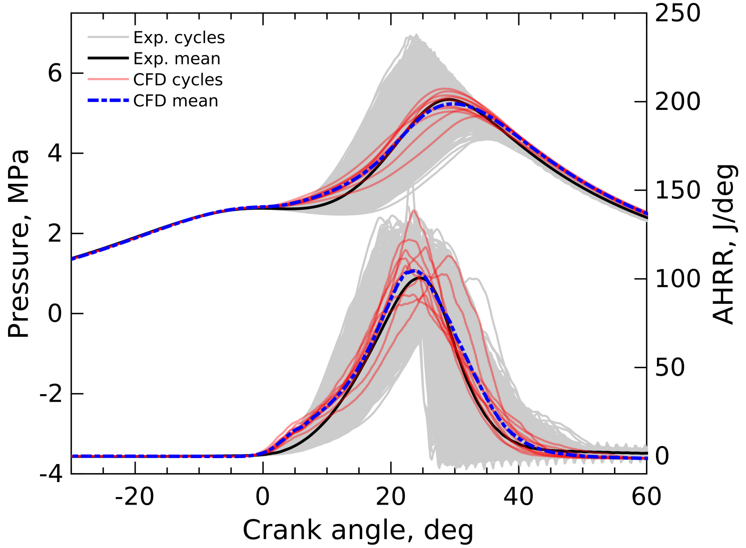
[1] Gao et al. Combust. Flame 167 (2016) 238-247
http://dx.doi.org/10.1016/j.combustflame.2016.02.007

Accomplishment | Baseline CFD performance established on success measures

Major Outcome 1

high load knock

S. Som (owner)

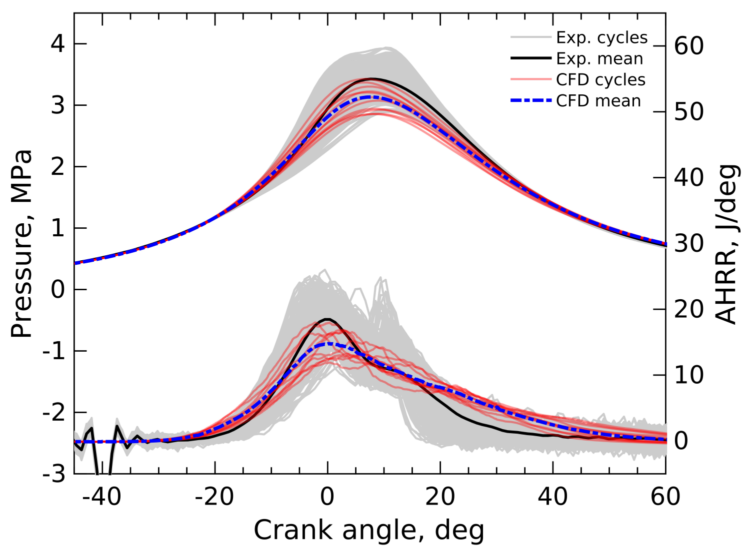


Target	Success	Baseline
KLSA	1 CAD	3 CAD
CPU cost	5x faster/5x more physics	---

Major Outcome 5

dilute cycle variability

M. Ameen (owner)

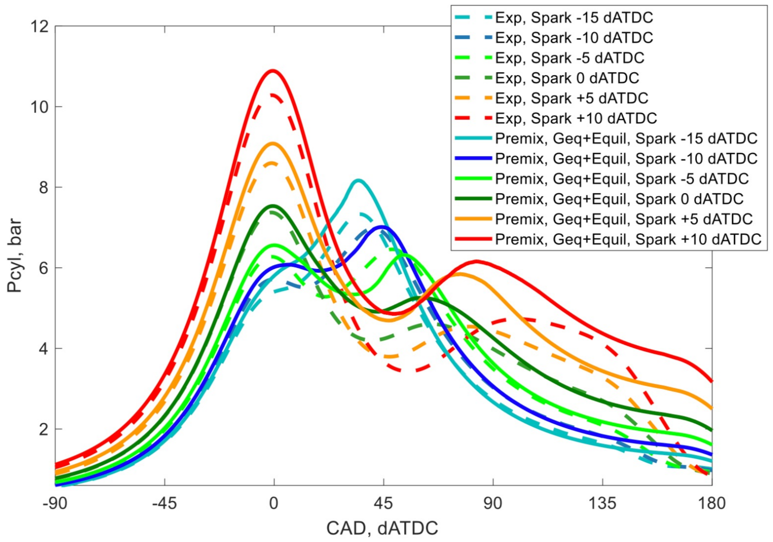


Target	Success	Baseline
COV	10%	100%
CA10-90	10%	36%

Major Outcome 8

cold start

K. D. Edwards (owner)



Target	Success	Baseline
COV	20%	No single param. set
Exhaust Enthalpy	10%	No single param. set
Emissions	20%	>1000% (soot*)

Success measures are for the predicted accuracy of the target for a design change with fixed model parameters.

* in canonical burners

PACE PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

Response to last year's reviewer comments (wt. avg. = 3.35/4)

- **Q1 Reviewer 5:** "*Delivering a usable, open-source product to OEMs is a key target… consider implementing technology transfer metrics into the program to track adoption*."

  The PACE leadership team has developed a "modeling menu" for the OEMs as part of our ongoing collaboration with the USDRIVE ACEC Tech Team. This document describes the features of more than 35 current sub-models, fuel mechanisms, tools, and best practices created or under development in the program that are available to the OEM and academic partners through PACE. It is a good idea to augment this document to include usage statistics by the OEMs for internal analysis and future reviews.

- **Q1 Reviewer 5:** "*[T]here will need to be close connection to, support from, and endorsement by engine manufacturers that the technologies being developed are of interest and have the potential to be commercially viable. Especially for novel combustion programs, such as Major Outcomes 5 and 7*"

  PACE removed Major Outcome 7 (low temperature gasoline combustion) and the lean ignition research in Major Outcome 5 to further increase the program's focus and speed development on the highest impact barriers for light-duty engines. The PACE leadership team is also actively helping the OEMs in the USDRIVE ACEC Tech Team to create the next roadmap extension for light-duty vehicle research.

- **Q1 Reviewer 5:** "*While recognizing that the move to a single engine platform may increase the speed to deliver modeling advancements, this reviewer was concerned that limiting to one engine design will impact the ability to deliver model validation. Improved, validated, modeling tools should be engine-agnostic and validated across a range of different engine platforms*"

  The PACE program will continue with two engines in FY22 at ANL, SNL and ORNL: the existing SG2, and the new PACE common platform. We agree that the modeling advancements should be independent of the engine. However, the benefit of learning simultaneously about sub-model performance on different experimental campaigns is too great given our mandate to move our research faster on a limited budget. The new platform will eliminate uncertainties attributed to different geometries and will increase confidence in the relevance of the models by predicting performance in a modern spark-ignition engine. Further, the success measures for Major Outcomes 1, 5, and 8 are for a blind prediction of a substantial design change, which forces the models to be as engine-independent as possible.

Program-Level Collaborations

- **USDRIVE ACEC Tech Team – invited PACE leadership to help create the next extension to the light-duty vehicle research roadmap**
- **Advanced Engine Combustion MOU partners**
  - Light-duty OEMs – Ford, General Motors, Stellantis (formerly FCA)
  - Heavy-duty OEMs – Caterpillar, Cummins, Daimler, GE, John Deere, Navistar, PACCAR, Progress Rail, Volvo, Wabtec
  - Energy companies – BP America, Chevron, ExxonMobil, Marathon, Phillips 66, Shell
  - Commercial CFD – ANSYS, Convergent Science, Gamma Tech., Siemens

Added FY20

- **Overlap and synergies with Co-Optima on a project level**
- **More than 50 additional project-level collaborations with U.S. and international universities and private/public research institutions**

Project-Level Collaborations

Manufacturers

Ford (2)
General Motors (5)
Hyundai
Stellantis
Toyota

Suppliers

Bosch
Bosch Motor Sports
Delphi
Hyundai KEFICO
Mahle
Tenneco
Transient Plasma Sys.

Software Vendors

ANSYS
AVL FIRE
Convergent Science (6)
Gamma Tech (2)
Pointwise
Siemens/StarCCM+

Fuels & Lubricants

Aramco
Chevron
Lubrizol

Research Councils

Comp. Chem. Consort.
Coordinating Research Council
IFP Energies Nouvelles
Inst. Motori (STEMS)

Universities

AIST, Japan
Auburn
City U. London
CMT U. Polit. Valencia
Colorado St.
Imperial College
Iowa St.
LTT Erlangen
KAUST (3)
Marquette U.
Michigan Tech.
Natl. U. Ireland – Galway
Polit. Milano
Princeton
RWTH Aachen
TU Darmstadt
UC Davis
U. Central Florida
U. Connecticut
U. Hawaii
U. Illinois U-C
U. Mass. Amherst
U. Mass Dartmouth
U. Sci. Tech. of China
U. Southern Calif.
U. Texas

Government

Army Research Laboratory

Remaining Challenges and Barriers

SPEED

- Coordinate PACE advances for +20 sub-models while evaluating their performance against four Major Outcomes (1, 4, 5 & 8) and prioritizing their future development with limited time and money.
- Leverage insight across different experimental campaigns simultaneously.

IMPACT

- Ensure that the proposed research can deliver significant efficiency gains (CO_2 savings), and emissions reductions.

ADOPT

- Accelerate knowledge and tool transfer to industry including the engine design workflows for the production engineers.

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

ADOPT IMPACT SPEED

- CFD Integration tasks for high-load knock (MO #1), dilute cyclic variability (MO #5), and cold start (MO #8) will report first integrated comparison of new PACE models at August AEC meeting
- Common PACE engines will be installed at ANL, SNL and ORNL
- PACE leadership team will help the OEMs develop the next ACEC Tech Team roadmap over the summer
- PACE simulation experts continue to update the public “modeling menu,” which contains +35 sub-models, mechanisms, tools, and best practices
  - and create a public website to connect stakeholders with the resources
- Zero-RK 3.0 release (planned for Aug. 2021) will include: simplified interface to link with CFD codes, mechanism optimization tools, counterflow diffusion flames, PSR, and IC engine models
  - and create common flame tables for the recommended PACE-20 mechanism

Summary

Relevance

- ICE powered vehicles will be a significant component of the US fleet for many decades
- Significant improvements in both emissions and efficiency are possible and needed to meet environmental goals

Approach

- The work plan for PACE is focused on three key areas and is developed in coordination with the USDRIVE ACEC Tech Team
- Coordinated collaborations across 7 Major Outcomes using kinetics, fundamental measurements and engine experiments feeding into improved models

Programmatic Accomplishments

- Purchased common PACE engine platform – single cylinder at ANL (metal) and SNL (optical), and single and multi at ORNL
- Recommended PACE-20 surrogate with more than a dozen new validation experiments
- Discontinued FY20 project to bolster investment in 4 areas: CFD integration tasks, spray models, new 500 bar injectors, and mechanism reduction tools
- Baseline CFD performance established on success measures for Major Outcomes 1, 5, and 8

Collaboration and Coordination

- PACE is a collaboration among five national laboratories working towards common objectives
- US DRIVE ACEC Tech Team, AEC MOU industry stakeholders, Commercial CFD, Co-Optima
- More than 50 project-level collaborations with U.S. and international universities and private/public research institutions

Proposed Future Research (any proposed future work is subject to change based on funding levels)

- Promoting closer coordination and increased relevance with a common, modern engine platform and gasoline surrogate
- Enhancing industry adoption of software and modeling tools by continually refining the hand-off with the ACEC tech team
- Building partnerships with other DOE offices on HPC, ML/AI, and Basic Energy Science

Technical Back-up Slides

Complete PACE Budget FY21

Code and Work Flow Development

		Lab	PI	FY20	FY21
A.M.05.01	Spray and Combustion model implementation	ANL	Ameen	350k	340k
A.M.05.02	Gridding, validation, and workflow development	ANL	Ameen	350k	300k
A.M.05.04	MO1 Integration	ANL	Som		75k
A.M.05.05	MO5 Integration	ANL	Scarcelli		75k
L.M.05.01	Accelerated multi-species transport in engine simulations	LLNL	Whitesides	275k	250k
L.M.05.02	Improved chemistry solver performance with machine learning	LLNL	Whitesides		250k
L.M.05.04	Scalable performance and CFD integration of ZERO-RK	LLNL	Whitesides	275k	75k
L.M.05.06	Mechanism Reduction	LLNL	Whitesides		75k
L.M.05.07	Accelerate Mechanism Reduction Tools	LLNL	Whitesides		75k

Cold Start

		Lab	PI	FY20	FY21
O.E.07	Multi-cyl Cold Start & surrogate testing	ORNL	Curran	350k	350k
S.E.07	Engine experiments characterizing wall films & PM formation	SNL	Sjoberg	270k	270k

Combustion and Emissions

		Lab	PI	FY20	FY21
O.E.02	Effectiveness of EGR to mitigate knock throughout PT domain	ORNL	Szybist	220k	175k
S.E.02	Experiments supporting particulate modeling -- wall film & pyrolysis	SNL	Manin	500k	400k
L.M.01	Improved Kinetics for Ignition Applications	LLNL	Pitz	150k	
S.M.02.01	DNS and modeling of turbulent flame propagation & end gas ignition	SNL	Chen	50k	50k
S.M.02.02	Flame wall interactions	SNL	Nguyen	150k	50k
S.M.02.03	Engineering PAH Model Development	SNL	Hansen		100k

Data Analytics

		Lab	PI	FY20	FY21
O.E.08	Machine Learning and Nonlinear Dynamics	ORNL	Kaul	200k	200k

Flows and Heat Transfer

		Lab	PI	FY20	FY21
O.E.06.01	Neutron diffraction for in situ measurements in an operating engine	ORNL	Wissink	100k	100k
O.E.06.02	Neutron Imaging of Advanced Combustion Technologies	ORNL	Wissink	200k	200k
O.M.06	Conjugate heat transfer	ORNL	Edwards	350k	350k
LA.M.06.01	Heat Transfer through Engine Metal - - -	LANL	Carrington	200k	
LA.M.06.02	Heat Mass Transfer in Liquid Species - - -	LANL	Carrington	200k	

Flows and Heat Transfer

		Lab	PI	FY20	FY21
O.E.06.01	Neutron diffraction for in situ measurements in an operating engine	ORNL	Wissink	100k	100k
O.E.06.02	Neutron Imaging of Advanced Combustion Technologies	ORNL	Wissink	200k	200k
O.M.06	Conjugate heat transfer	ORNL	Edwards	350k	350k
LA.M.06.01	Heat Transfer through Engine Metal - - -	LANL	Carrington	200k	
LA.M.06.02	Heat Mass Transfer in Liquid Species - - -	LANL	Carrington	200k	

Fuel Kinetics and Surrogates

		Lab	PI	FY20	FY21
A.E.01	Measurements of autoignition fundamentals at dilute gasoline conditions	ANL	Goldsborough	280k	252k
L.M.01	Surrogates and Kinetic Models	LLNL	Pitz	500k	425k
L.M.01.02	Models for improved prediction of PAH/soot	LLNL	Kukkadapu	200k	200k

Ignition

		Lab	PI	FY20	FY21
A.M.03	Advanced Ignition Modeling Tools	ANL	Scarcelli	400k	370k
N.M.03	ML based LES ignition model	NREL	Yellapantula	275k	275k
S.M.03.01	DNS of early ignition kernel development	SNL	Chen	100k	100k
S.M.03.02	Physics based flame-kernel LES modeling	SNL	Nguyen	100k	100k
A.E.03	Fundamental Ignition Experiments	ANL	Rockstroh	380k	342k
S.E.03.01	Advanced Ignition to Enable Alternative Combustion Modes	SNL	Ekoto	420k	420k
S.E.03.02	Fundamental ignition experiments	SNL	Ekoto	420k	420k

LSPI

		Lab	PI	FY20	FY21
O.E.09.01	Fuel spray wall wetting and oil dilution impact	ORNL	Splitter	220k	220k

Sprays

		Lab	PI	FY20	FY21
A.E.04	X-Ray Studies of Fuel Injection and Sprays	ANL	Powell	490k	441k
O.E.04.01	Injector Characterization & Distribution	ORNL	Wissink		125k
S.E.04	Spray Experiments	SNL	Pickett	380k	380k
S.E.04.03	GDI sprays leadership & data sharing	SNL	Pickett	140k	140k
A.M.04	Towards Predictive Simulations of Sprays in Engines	ANL	Torelli	300k	220k
A.M.04.01	Improved free spray and spray-wall interaction modeling	ANL	Torelli		125k
LA.M.04.01	Simulate free sprays in chamber and engines - - -	LANL	Carrington	200k	
S.M.04.01	Free spray modeling	SNL	Nguyen	50k	50k
S.M.04.02	Free spray modeling addition	SNL	Tagliente		125k

Response to last year's reviewer comments (wt. avg. = 3.35/4)

- **Q3 Reviewer 4:** *"With regards to cold-start emissions, the reviewer would have liked to see more information on how PACE will collaborate with aftertreatment research teams"*

  The PACE leadership and the CLEERS (Crosscut Lean Exhaust Emissions Reduction Simulations) leadership have started this year coordinating with the OEM members of the USDRIVE ACEC Tech Team. The goals are to define the simulation outputs needed from PACE and the the aftertreatment model in order to predict tailpipe emission.

- **Q4 Reviewer 3:** *"… the major outcomes are not overly specific as to what final success looks like… More clarity is necessary to define a quantifiable result state, which could be considered a success"*

  All the major outcomes have a success measure that can be computed and validated against engine experiments. The success measures for Major Outcomes 1, 4, 5, and 8 are based on a priori prediction accuracy of an engine design change (geometry or operating conditions). Major Outcomes 2, 3, and 6, have success measures based on the experimental demonstration of a specific aspect of engine performance. In all cases, the quantifiable level to declare success is based on detailed feedback from the ACEC Tech Team each year.

Response to last year's reviewer comments (wt. avg. = 3.35/4)

- **Q4 Reviewer 4:** "*The use of artificial intelligence (AI) and machine learning (ML) should be handled carefully… Machine learning should be used to handle turnaround time*."

  The ML based models developed at NREL have been designed to complement the physics-based models. The starting point for all the ML based models are state-of-the-art (SOA) physics-based models and are designed to reproduce the asymptotic behavior of physics-based models. We also tightly couple various physics-based realizability conditions during the ML model development process. In terms of testing to establish confidence in these ML based models, the team at NREL has been performing blind validation tests against the DNS data and in FY21-FY22 we plan to perform a-posteriori tests against experimental data. Additionally, these ML based models are also designed to efficiently utilize higher computing power afforded by the latest supercomputing technologies.

- **Q4 Reviewer 5:** "*the reviewer still would have liked to see some additional information on the codes that will be used for the direct numerical simulations (DNS). Why are these codes needed if the ultimate goal is to get the models in commercial codes used by the OEMs?*"

  There are two ASCR-funded codes in the Exascale Computing Project that are used in the PACE program - NEK5000 and Pele. NEK5000 is needed to provide the highest fidelity turbulence resolution of all the in-cylinder flow processes (both non-reacting and reacting) using high-order, large eddy simulation (LES). The availability of such resolution allows the CFD integration tasks for Major Outcome 1 (high load knock) and Major Outcome 5 (dilute cyclic variability) to establish the best performance available on the success measures, and to isolate numerical errors in the flow-field coupling versus the standalone sub-models for other physical processes. Pele is capable of performing direct numerical simulation (DNS) of reacting flows but cannot simulate the entire cylinder during the full reacting cycle even with a complete takeover of the DOE's largest supercomputer. As such, it will be used as a microscope to investigate fundamental turbulent-combustion processes not currently resolved in engineering models with the aim of developing better sub-models for early flame kernel development, end-gas auto-ignition, and flame-wall interactions.

Abbreviations

ACEC	Advanced Combustion & Emissions Control
AEC MOU	Advanced Engine Combustion Memorandum of Understanding
AI	Artificial Intelligence
AMR	Annual Merit Review
ANL	Argonne National Laboratory
APS	Advanced Photon Source
ASCR	Advanced Scientific Computing Research
AVL	Anstalt für Verbrennungskraftmaschinen List GmbH
BOB	Blendstock for Oxygenate Blending
CA/CAD	Crank Angle in Degrees
CFD	Computational Fluid Dynamics
COV	Coefficient Of Variation
CPU	Computer Processing Unit
DOE	Department of Energy
EGR	Exhaust Gas Recirculation
EIA	U.S. Energy Information Administration
EPA	Environmental Protection Agency
FY	Fiscal Year
GE	General Electric
HPC	High Performance Computing
ICE	Internal Combustion Engine
KLSA	Knock Limited Spark Advance
LLNL	Lawrence Livermore National Laboratory
LSPI	Low Speed Pre-Ignition
ML	Machine Learning
MO	Major Outcome
NREL	National Renewable Energy Laboratory
OEM	Original Equipment Manufacturer
ORNL	Oak Ridge National Laboratory
PACE	Partnership for Advanced Combustion Engine
PI	Principal Investigator
RCM	Rapid Compression Machine
SNL	Sandia National Laboratories
SNS	Spallation Neutron Source
UDF	User Defined Function
VOF	Volume of Fluid
VTO	Vehicle Technologies Office