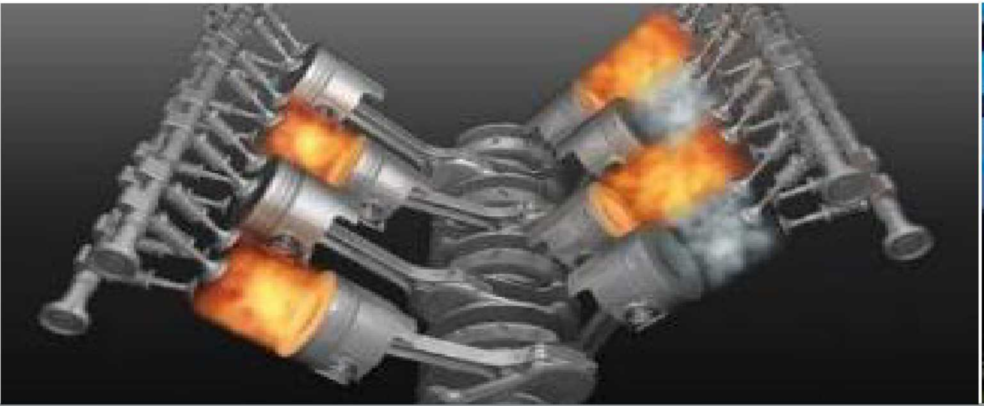
SAND2020-4498PE

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

Matthew McNenly, Paul Miles*, Sibendu Som, Jim Szybist

*Presenter

Annual Merit Review, 2 June 2020, 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: ~25%

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 FY20 budget $9125K
- Approximate allocations
  - Knock/LSPI mitigation ~ 32%
  - Dilute combustion ~ 31%
  - Emissions reduction ~ 37%

Budget breakdown by task provided in reviewer only slides

Partners

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

Project leads

- Matt McNenly (LLNL)
- Paul Miles (SNL)
- Sibendu Som (ANL)
- Jim Szybist (ORNL)

Program-Level Collaborations

- **USDRIVE ACEC Tech Team**
- **Advanced engine combustion MOU partners**
  - Light-duty OEMs – Fiat Chrysler, Ford, General Motors
  - 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, Converge CFD, Siemens **New this year**
- **Overlap and synergies with Co-Optima on a project level**
- **Numerous additional project-level collaborations with U.S. and international universities and private/public research institutions**

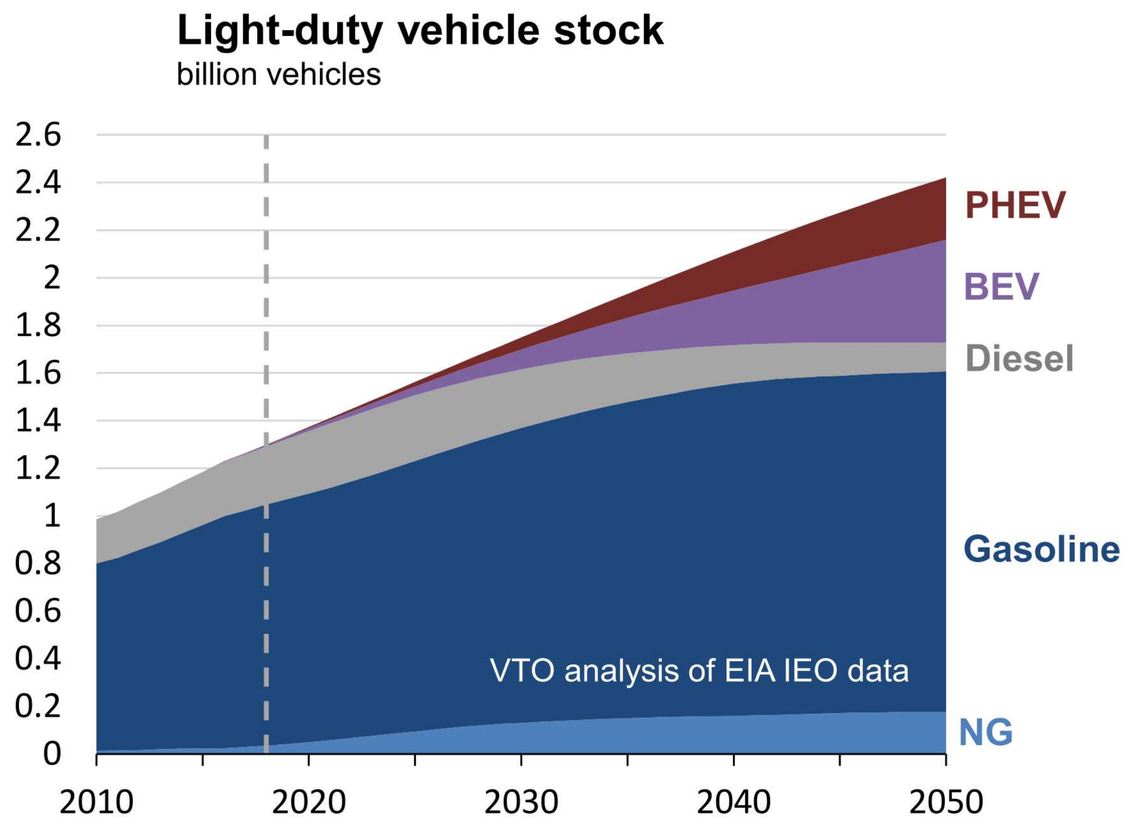
Relevance | Improved ICEs are key to energy and environmental security

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

2019 International Energy Outlook, EIA

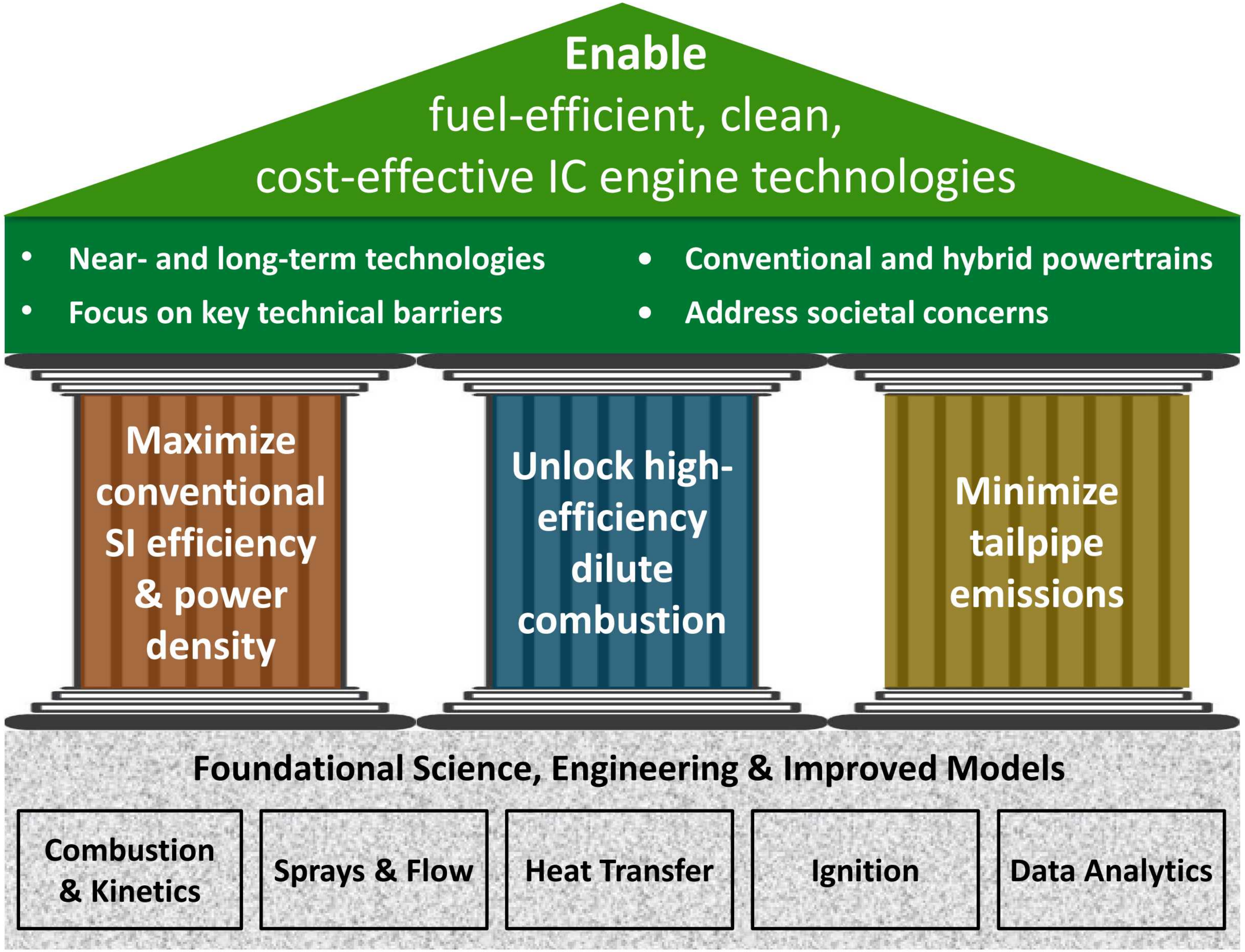


PACE PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

Relevance | Research is focused on key priorities

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 | Each key area directly impacts energy and environmental security

Maximize conventional SI efficiency & power density

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

Unlock high-efficiency dilute combustion

- **Highest potential efficiency gains but significant barriers**
  - Mid-term, high EGR stoichiometric for > 12% efficiency gain
  - Long-term, lean combustion for ~ 25% efficiency gain

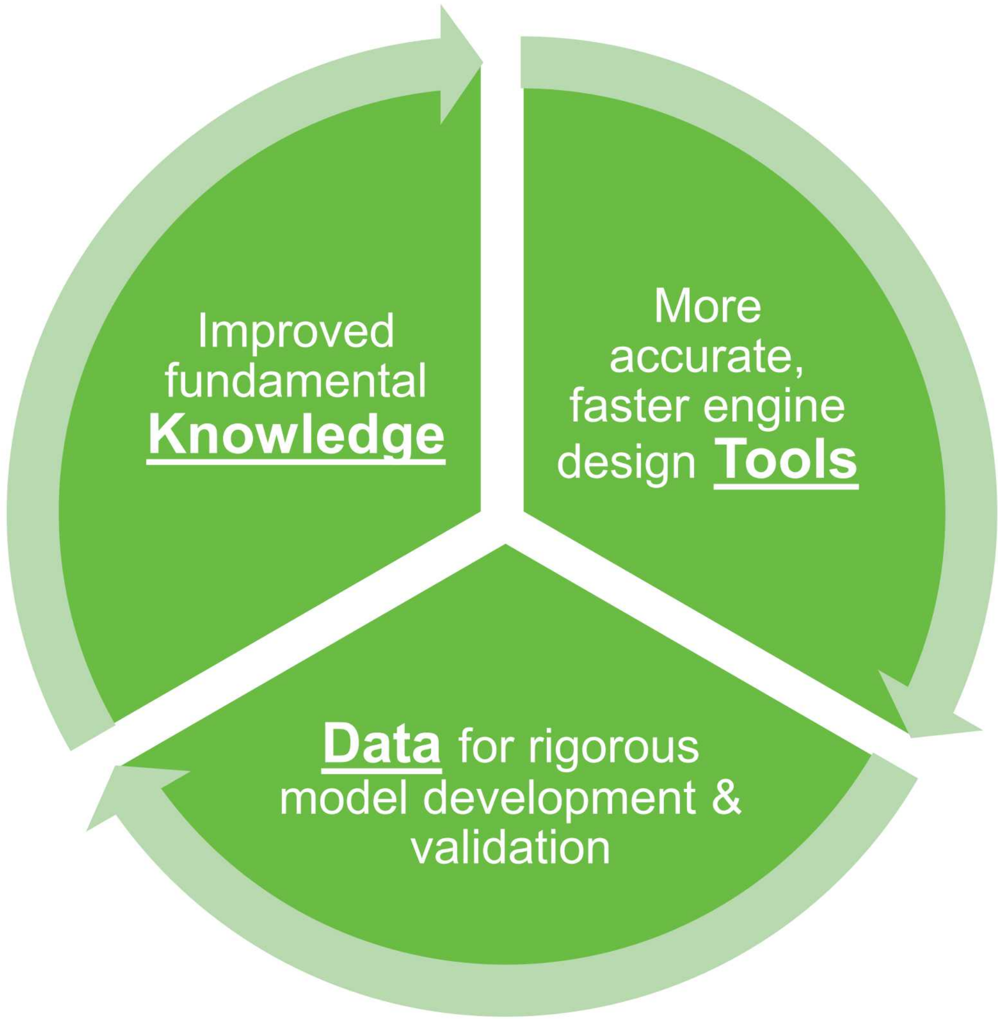
Minimize tailpipe emissions

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

Approach | Accelerated, more accurate engine design for sustainable transportation

PACE combines unique experiments with world-class DOE computing and machine learning expertise to

- **speed** discovery of knowledge
- **improve** engine design tools
- **enable** market-competitive powertrain solutions

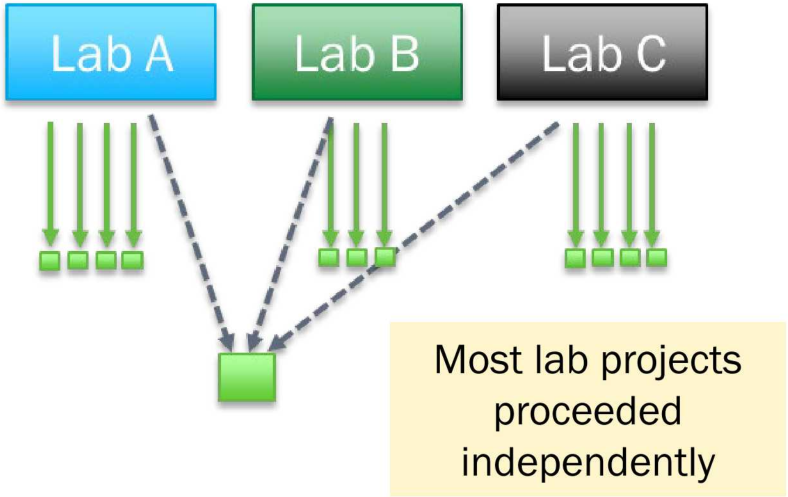


Approach | Tighter inter-laboratory collaborations

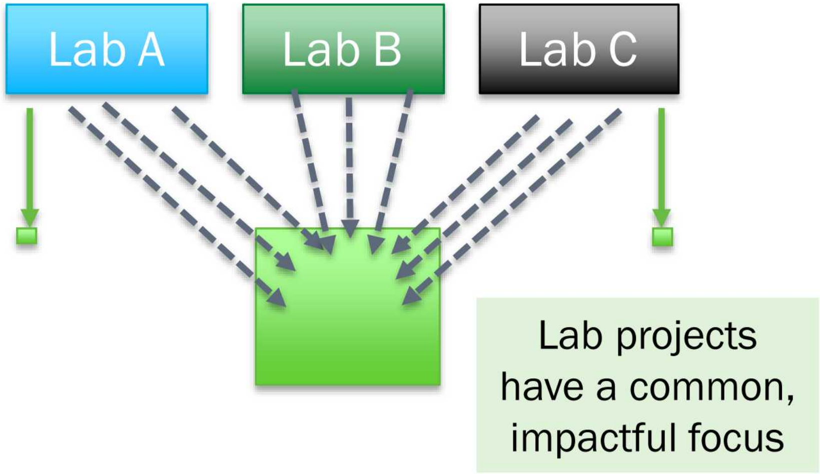
To revolutionize global trade…

… it took the right level of organization

Before

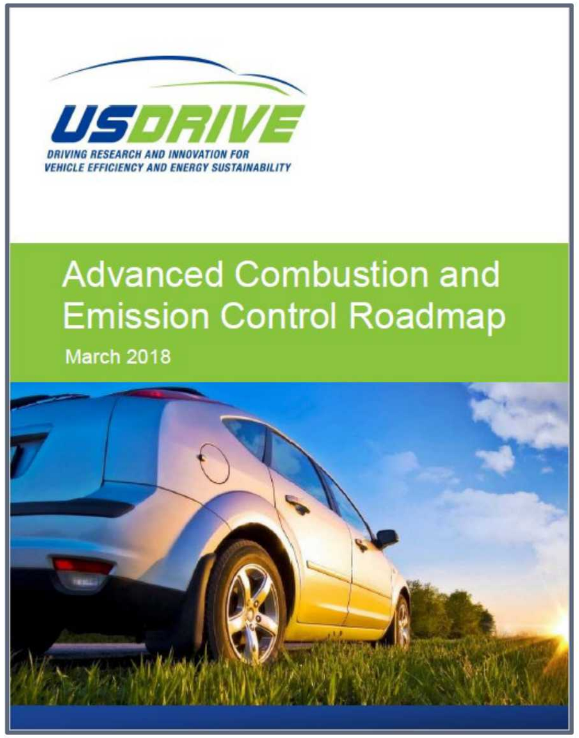


PACE



Approach | Work tightly aligned with OEM priorities and workflows

- Strong alignment with USDRIVE ACEC Tech Team priorities
- *Ab initio* engagement on work planning



PACE

Open source models

ANSYS

CONVERGE

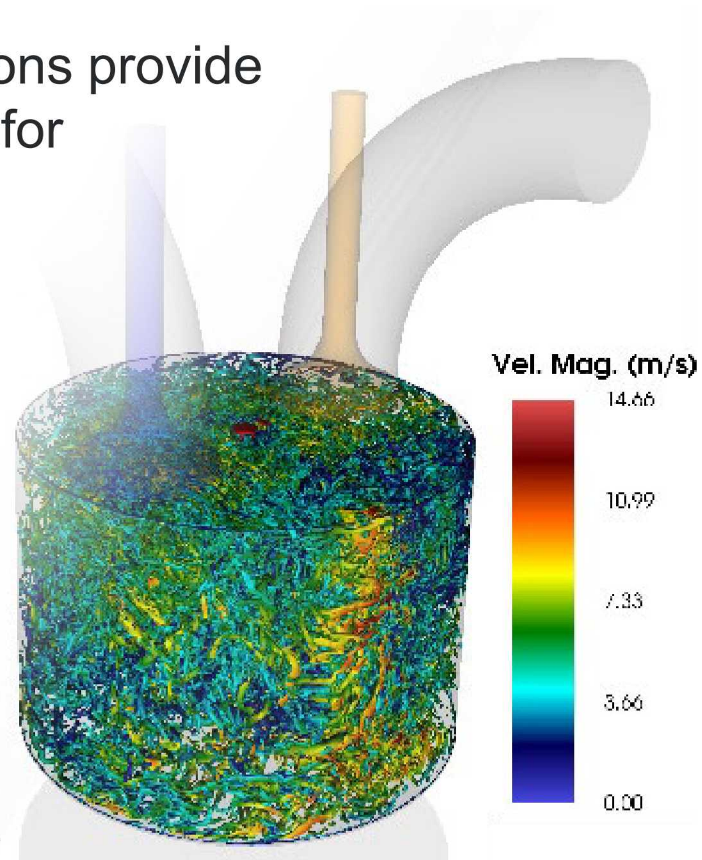
SIEMENS

Everyone is 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)
  - Create efficient ‘surrogate’ models for engine multi-parameter optimization
  - Develop expert systems enabling optimal CFD-based design
  - Develop data-driven efficient sub-models

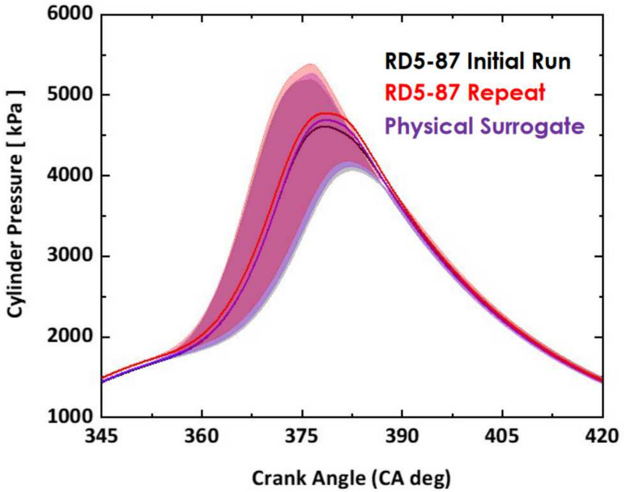
www.anl.gov/es/article/transforming-transportation-with-machine-learning

Accomplishments | All tasks support 8 Major Outcomes

Major Outcome 1:

Source: ORNL

Accurately predict knock response to design changes

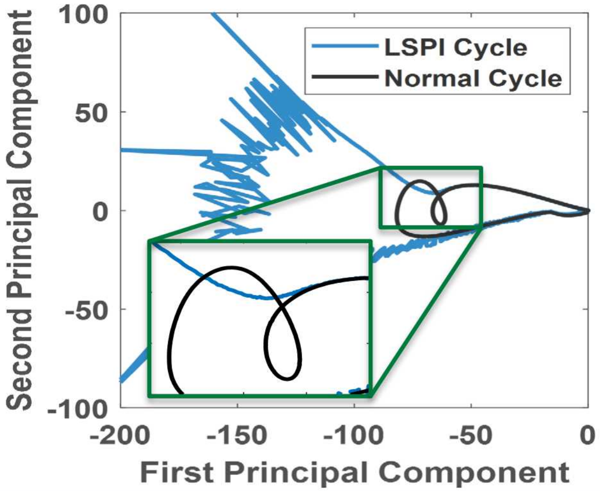


Major Outcome 2:

Source: ORNL

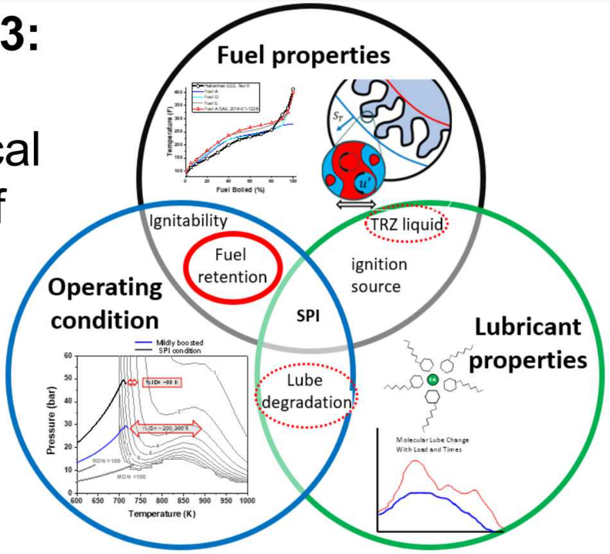
Data analytics detect & control knock/LSPI

PCA allows earlier detection than conventional pressure analysis



Major Outcome 3:

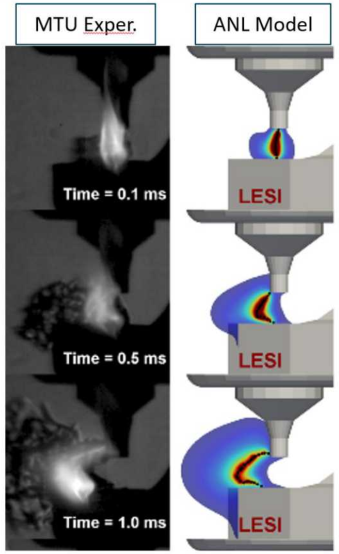
Phenomenological understanding of LSPI identifying pathways for mitigation



Source: ORNL

Major Outcome 4:

Improved ignition modeling enabling better igniter high-load performance



Source: ANL

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 KLSA within 1 degree over the knock-limited operating range of the engine, with a 5X reduction in simulation time

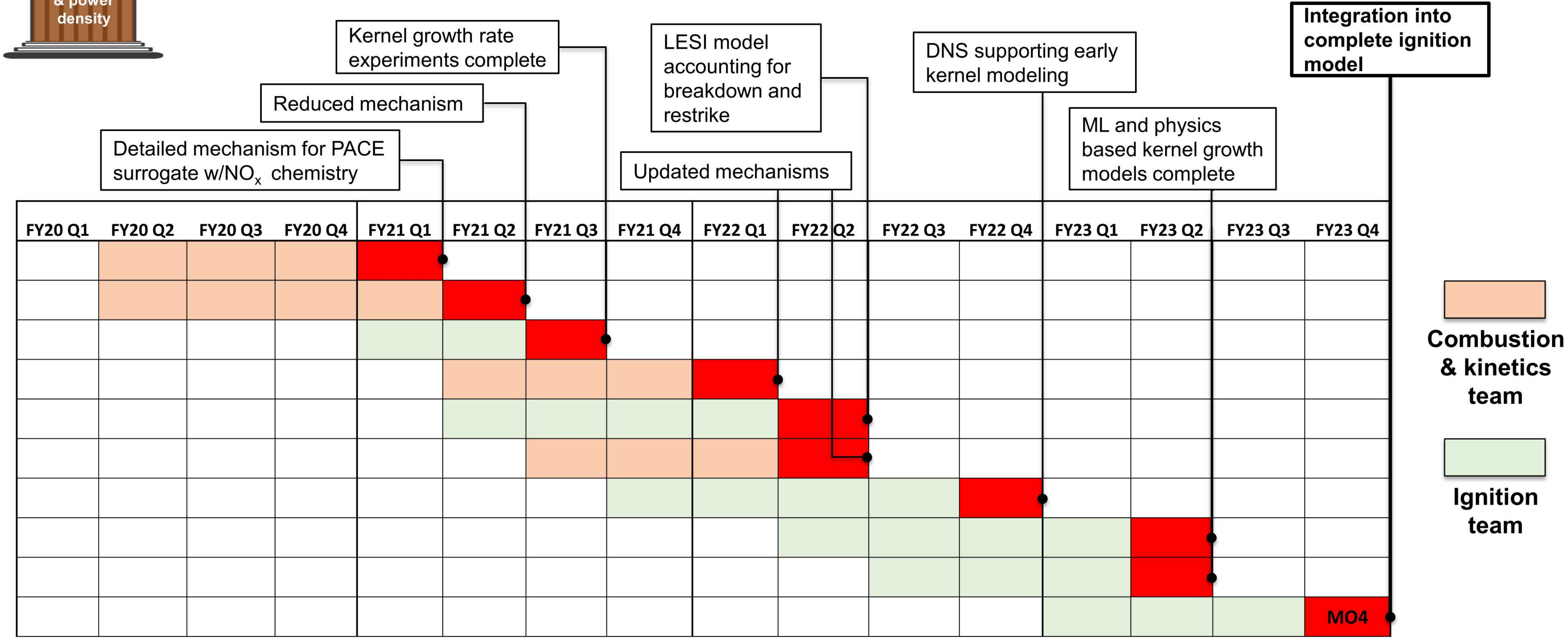
Major Outcome 2: Data analytics enable operation and real-time control to mitigate knock/LSPI

Success measure:

Use advanced data analytics to identify knock propensity and control using existing or future sensors to make 100% of cycles run at KLSA or MBT

Example Milestones | Each major outcome has associated key intermediate milestones and a timeline defined

Major Outcome 4: Improved ignition modeling enabling better igniter high-load performance and durability

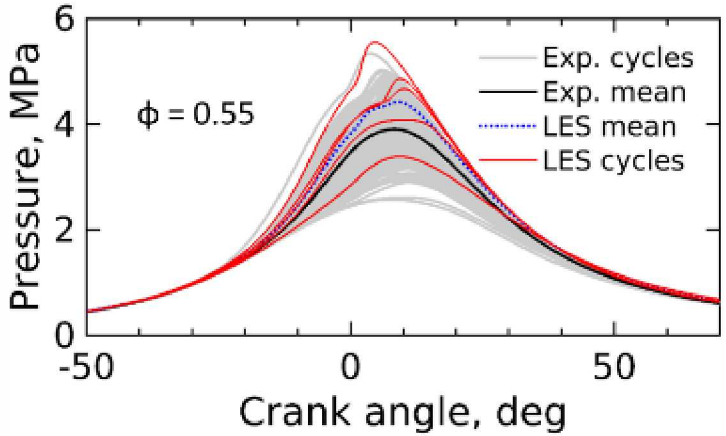


Accomplishments | All tasks support 8 Major Outcomes

Major Outcome 5:

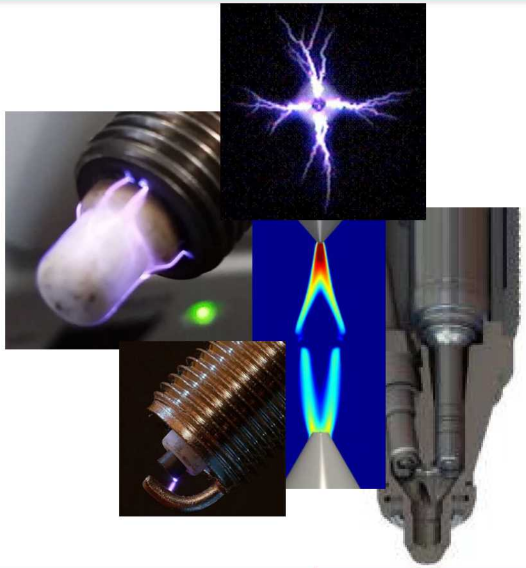
Source: ANL/SNL

Predictive modeling of dilute engine efficiency and emissions



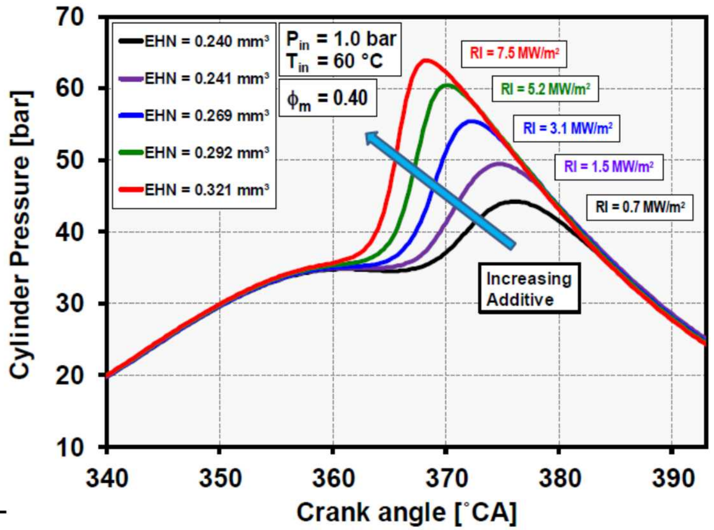
Major Outcome 6: Advanced igniters and control methods that expand existing dilution limits

(also couples to improved cold-start)



Major Outcome 7:

Next-cycle phasing and stability control for gasoline CI combustion

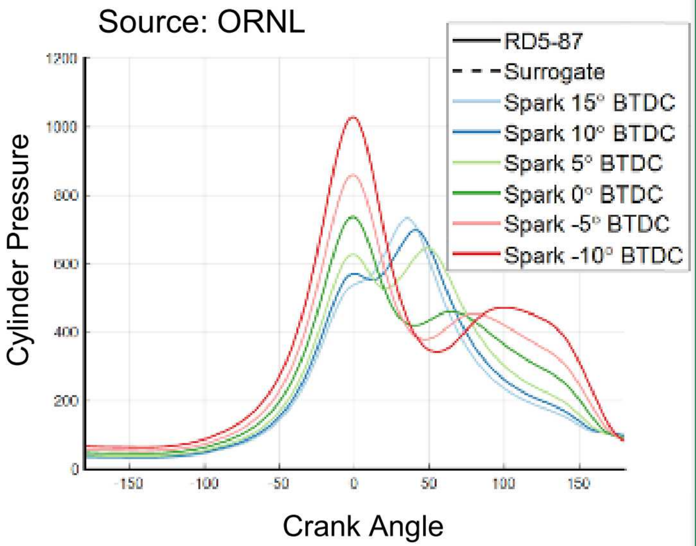


Source: SNL

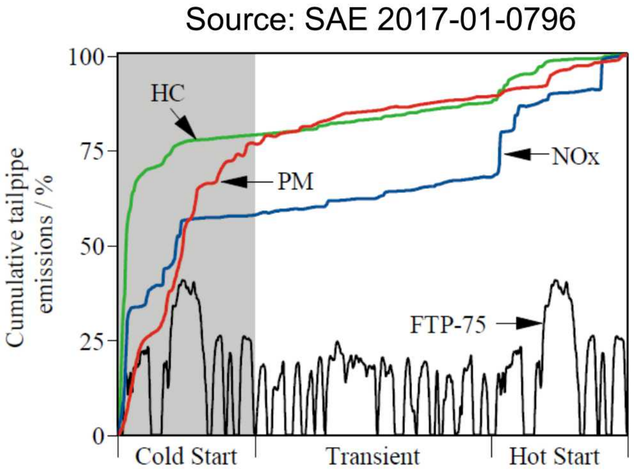
Accomplishments | All tasks support 8 Major Outcomes

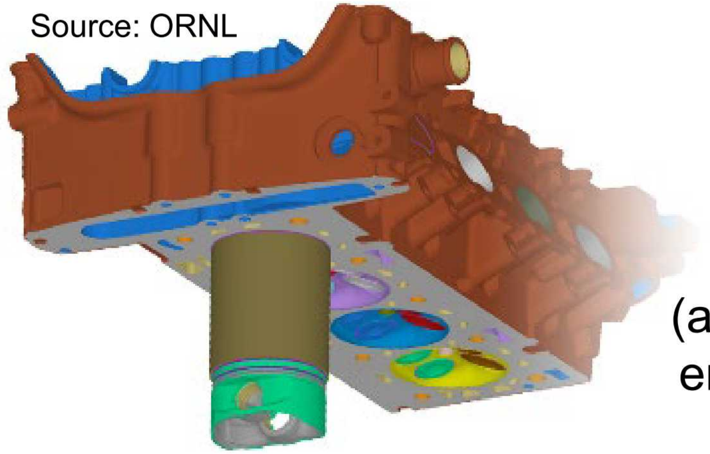
Major Outcome 8

Predictive modeling of in-cylinder combustion phasing and stability



Predictive modeling of engine-out cold-start emissions

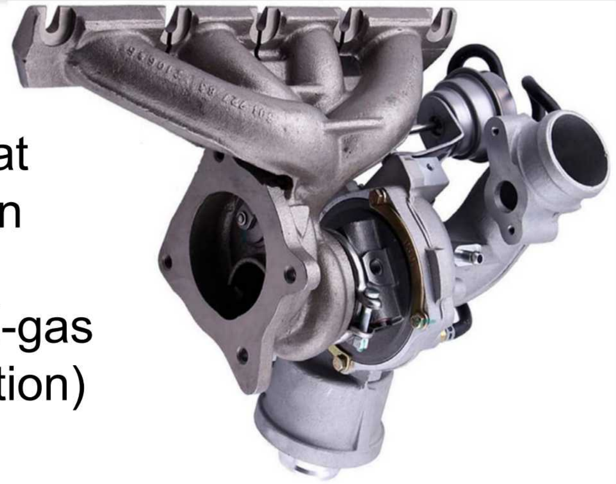




Simulations of CHT for full multi-cylinder engine including exhaust system

Exhaust system heat losses and oxidation

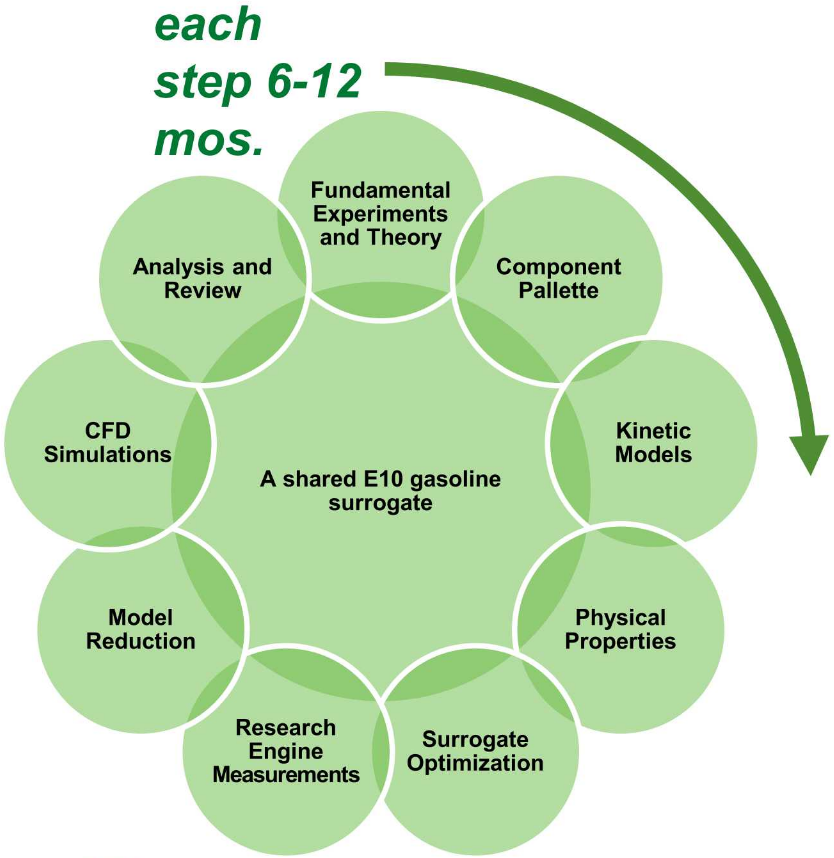
(accurate catalyst feed-gas enthalpy and composition)



Fully instrumented exhaust for temperature and species

Early accomplishment | The surrogate team was formed to rapidly establish a well-characterized, full boiling range surrogate fuel

- Surrogate fuels used for simulation have typically been very simple – PRF or TRF mixtures
  - Able to match autoignition characteristics, but not other parameters important to mixture preparation and combustion
- Under PACE, we seek to develop a tractable surrogate that can be for multiple aspects of engine design
- Both chemical and physical properties much be matched
  - RON/MON
  - H:C ratio
  - Carbon type & #
  - Flame speed
  - Heat of Vaporization
  - Distillation curve
  - PMI
  - Viscosity
  - Surface Tension
  - Density
  - LTHR/ITHR
  - & etc.



How do we increase the PACE?

Iterative development cycle would leave us with dozens of mismatched palettes, blends, chemistry models, and reductions over the next 5 years

Early accomplishment | A viable surrogate for initial SI and cold-start simulations has been developed and tested in just 3 months

Experiments	RD5-87	PACE-01	PACE-02	PACE-03	PACE-04	PACE-05	PACE-06	PACE-07	PACE-08	PACE-09	PACE-10	PACE-11	PACE-12	PACE-13	PACE-14	PACE-15	PACE-16	PACE-17
RON	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
MON	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
D86	X	X			X					X	X	X	X	X	X			
DHA	X	X								X								
ADC	X																	
Flame Speed	X																	
Boosted SI	X	X																
Cold Start	X	X																
Cold Start (PM)	X	X																
LTHR/ITHR (NA)	X	X																
LTHR/ITHR (boosted)	X	X			X													

- Working together, in three months time we have:
  - Developed blending protocols
  - Tested 17 fuels for RON/MON and other properties, achieving excellent matches for several fuels
  - Significantly enhanced our modeling of RON/MON for tuning future surrogate candidates

- Engine validation of one surrogate in boosted SI (ACE147) and cold-start tests (ACE149) reproduced KLSA and cold-start combustion performance and gaseous emissions very well
- Additional work is needed to capture cold-start PM and autoignition reactivity under LTC conditions

PACE PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

Programmatic level future capabilities and collaborations

Engine modernization & standardization

- Different engine facilities in the national laboratories impede close collaboration
- Engines may not represent modern, fast-burn combustion systems
- Implement a common platform enabling data, understanding, and models to be developed under conditions close to next generation engines:
  - Single-cylinder test engines at ORNL/ANL
  - Optical single cylinder engine at SNL
  - Multi-cylinder engine at ORNL
- In consultation with the ACEC Tech Team have selected the Ford 2.3 liter engine as the baseline production engine

Machine Learning subprogram (ML4ICE)

- Closer cooperation with Office of Science (SC) programs
  - Leverage software/hardware investments
  - Access scientific ML expertise (SciDAC)
    - domain aware (respect laws of physics)
    - interpretable (explain model decisions)
    - robust (stable & reliable with real data)
- Perform “gold standard” calculations by bringing highest-fidelity simulations possible to train engineering level models
- Speed progress by creating an ecosystem for ML experts to work with ICE experts
- Connect with data science centers across the national labs to design data campaigns and mentor projects

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

PACE talks in this session

Title	Presenter	Presention ID
PACE - a Light-duty National Laboratory Combustion Consortium	Paul Miles (SNL)	ACE138
Development of an Optimized Gasoline Surrogate Formulation for PACE Experiments and Simulations	Scott Wagnon (LLNL)	ACE139
Improved Chemical Kinetics and Algorithms for More Accurate, Faster simulations	Russell Whitesides (LLNL)	ACE140
Advanced Ignition System Fundamentals, Isaac Ekoto, SNL	Isaac Ekoto (SNL)	ACE141
Development and Validation of Simulation Tools for Advanced Ignition Systems	Ricardo Scarccelli (ANL)	ACE142
Fuel Injection and Spray Research	Chris Powell (ANL)	ACE143
Spray Wall Interactions and Soot Formation	Lyle Pickett (SNL)	ACE144
Direct Numerical Simulation (DNS) and High Fidelity Large Eddy Simulation (LES) for Improved Prediction of In Cylinder Flow and Combustion Processes	Muhsin Ameen (ANL)	ACE146
Mitigation of Knock and LSPI for High-Power Density Engines	Jim Szybist (ORNL)	ACE147
Overcoming Barriers for Dilute Combustion	Brian Kaul (ORNL)	ACE148
Cold-Start Physics and Chemistry in Combustion Systems for Emissions Reduction	Scott Curran (ORNL)	ACE149
More Accurate Modeling of Heat Transfer in Internal Combustion Engines	Dean Edwards (ORNL)	ACE145

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 Outcome 8 using kinetics, fundamental measurements and engine experiments feeding into improved models
- We are incorporating DOE advances and expertise in HPC and ML/AI to speed progress

Programmatic Accomplishments
- Focused all tasks on eight major outcomes supporting OEM research priorities
- Achieved unparalleled cooperation among the participating laboratories
- Early technical successes in surrogate fuel development demonstrate effectiveness of approach

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

Proposed Future Research*
- Promoting closer coordination and increased relevance with modern common engine platform
- Coherent 5-year research plan developed
- Building partnerships with other DOE offices on HPC and ML/AI

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

Technical back-up slides

Accomplishments | All tasks support 8 Major Outcomes

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: *Use advanced data analytics to identify knock propensity and control using existing or future sensors to make 100% of cycles run at KLSA or MBT*

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% eliminate the occurrence of LSPI*

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

Success measure: *Achieve a 50% reduction of kernel extinctions and restrikes at high-load conditions by Predictive ignition models, including spark plug geometry and electrical discharge circuit, that can be used to predict spark stretch, flame initiation, spark blowout and restrike, and spark discharge voltage and current. Accurately predict 0-5% mass burned fraction within 10% (mean and standard deviation)*

Accomplishments | All tasks support 8 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

<u>Success measure</u>: *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

<u>Success measure</u>: *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: Next-cycle phasing and stability control methods for lean/dilute compression ignition combustion strategies that respect noise and emissions limits

<u>Success measure</u>: *Combustion phasing control to within ±1° demonstrated over a load transient of 100 $N\text{-}m\text{-}s^{-1}$ and a pathway identified for control to 200 $N\text{-}m\text{-}s^{-1}$, with COV in IMEP < 3% at key steady-state operating points*

Minimize tailpipe emissions

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.

Reviewer only slides

Critical Assumptions & Issues

- 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

Complete PACE Budget

Combustion and Kinetics Team

		Lab	PI	FY19	FY20
A.01.01	Improve kinetic models for gasoline surrogates for combustion control, cyclic variability, and emission reduction	LLNL	Pitz	$325k	
A.01.02	Improved Kinetics for Ignition Applications	LLNL	Pitz		$150k
A.01.03	Kinetic models for improved prediction of PAH/soot for emission reduction	LLNL	Pitz		$200k
A.01.04	Kinetic models with improved EGR behavior for impact on cyclic variability and combustion control	LLNL	Pitz		$200k
A.01.05	New/improved kinetic models for gasoline components for emission reduction, combustion control and cyclic variability	LLNL	Pitz		$150k
A.02.01	Accelerated multi-species transport in engine simulations	LLNL	Whitesides		$275k
A.02.02	Improved chemistry solver performance with machine learning	LLNL	Whitesides	$175k	
A.02.04	Scalable performance and CFD integration of ZERO-RK	LLNL	Whitesides		$275k
A.02.05	Towards exa-scale combustion simulations with real fuel kinetics	LLNL	Whitesides	$150k	
A.03.01	Autoignition fundamentals at dilute gasoline conditions	ANL	Goldsborough	$450k	$450k

Heat Transfer Team

		Lab	PI	FY19	FY20
B.01.01	Neutron diffraction for in situ measurements in an operating engine	ORNL	Wissink	$1057k	$100k
B.01.03	Heat Mass Transfer in Liquid Species	LANL	Carrington	$200k	$200k
B.02.01	Accelerating predictive simulation of internal combustion engines	ORNL	Edwards	$200k	$400k

Ignition and Kernel Formation Team

		Lab	PI	FY19	FY20
C.01.01	Advanced Ignition to Enable Alternative Combustion Modes	SNL	Ekoto	$370k	$420k
C.01.02	Fundamental experiments of ignition	SNL	Ekoto	$100k	$420k
C.02.01	SNL DNS/Modeling – Dilute spark ignition	SNL	Chen	$50k	$100k
C.02.02	ML-based Ignition Model Process Development	NREL	Grout		$275k
C.02.03	Turbulence Chemistry Interaction and Ignition Modeling	SNL	Nguyen	$80k	$100k
C.02.04	Development/validation of simulation tools for advanced ignition systems	ANL	Scarcelli	$400k	$400k

Sprays and Wall Films

		Lab	PI	FY19	FY20
D.01.01	Studies of fuel injection for LD Engines	ANL	Powell	$200k	$200k
D.01.02	Neutron Imaging of Advanced Combustion Technologies	ORNL	Wissink	$50k	$200k
D.01.03	Droplet Dynamics	SNL	Dahms	$200k	$100k
D.01.04	GDI Particulates	SNL	Skeen	$570k	$500k
D.01.05	GDI spray effects on cyclic variability and cold start	SNL	Pickett	$380k	$380k
D.01.06	GDI sprays leadership & data sharing	SNL	Pickett	$140k	$140k
D.02.01	Towards predictive simulations of GDI Sprays	ANL	Torelli	$300k	$300k
D.02.02	Simulate free sprays in chamber and engines	LANL	Carrington	$200k	$200k
D.02.03	SNL Modeling – Simulations of Wall Wetting and Soot Formation	SNL	Nguyen	$100k	$100k
D.02.04	VOF Simulations Spray G	LANL	Carrington	$200k	$200k

Lean and Dilute Combustion

		Lab	PI	FY19	FY20
F.01.01	Multimode combustion in LD SI Engines	ANL	Rockstroh	$600k	$600k
F.01.02	Effectiveness of EGR to mitigate knock throughout PT domain	ORNL	Szybist	$125k	$220k
F.01.03	Fuel spray wall wetting and oil dilution impact on LSPI	ORNL	Splitter	$100k	$220k
F.02.01	Developing a framework for performing high-fidelity engine simulations using Nek5000 code	ANL	Ameen	$700k	$700k
F.02.02	Multimode combustion phasing control	SNL	Dec	$280k	$280k

Emissions Reduction

		Lab	PI	FY19	FY20
E.01.01	SI Cold Start	ORNL	Curran	$125k	$350k
E.01.02	Spray flow interaction, mixture formation, and combustion in an optical DISI Engine	SNL	Sjoberg	$270k	$270k
E.02.01	DNS/Modeling of soot emissions from wall films during cold-start and for fuel efficient lean/dilute stratified SACI-like combustion	SNL	Chen	$50k	$100k

Crosscutting

		Lab	PI	FY19	FY20
G.02.01	Machine learning and deterministic patterns	ORNL	Kaul	$150k	$200k