Cold-start Modeling and Experiments for Emissions Reduction (ACE 145)

K. Dean Edwards, Martin Wissink, Gurneesh Jatana, Flavio Chuahy, Scott Curran

Oak Ridge National Laboratory

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This research was conducted as part of the Partnership to Advance Combustion Engines (PACE) sponsored by the U.S. Department of Energy (DOE) Vehicle Technologies Office (VTO). A special thanks to DOE VTO program managers Mike Weismiller and Gurpreet Singh.

Overview

Timeline

- **PACE started FY2019 Q3**
- **Proposed as 5-yr project under DOE lab call (~45% complete)**
  - Focus and objectives of tasks will be adjusted
- **Overall PACE work plan discussed in ACE 138**

FY2019	FY2020	FY2021	FY2022	FY2023

Budget

PI	Task	FY2019	FY2020	FY2021
Wissink (ORNL)	O.E.06.01 Neutronic engine	$1009k*	$100k	$100k
Jatana (ORNL)	O.E.07 Multi-cylinder Cold-start testing	$125k	$350k	$350k
Edwards (ORNL)	O.M.06 Cold-start simulation efforts	$200k	$350k	$350k

* One-time funding for hardware purchase

Barriers

- **U.S. DRIVE Advanced Combustion and Emission Control Roadmap**
  - Understand and improve dilute combustion strategies during *cold-start and cold operation to reduce emissions*.
  - *Understanding and robust modeling tools* for rapidly screening proposed designs based on sound metrics are lacking.
- **PACE Major Outcome 8**
  - Deeper understanding of *cold-start physics and chemistry* to enable *faster, numerically aided design and calibration*.

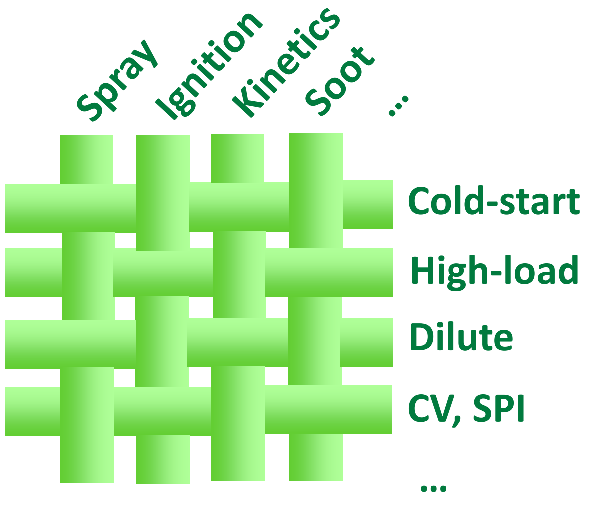
Partners

- **PACE is a DOE-funded consortium of 5 National Labs working toward common objectives (ACE 138)**
  - Goals and work plan developed with input from stakeholders including DOE, ACEC Tech Team, commercial CFD vendors, et al.
- **Specific partners on the work shown here…**
  - Wissink: *Providing validation data* to PACE modeling teams; SwRI, ORNL Spallation Neutron Source (SNS) and Neutron Sciences Directorate
  - Jatana: *Providing validation data* to PACE modeling teams
  - Edwards: *Receiving data and submodels* from PACE teams; Convergent Science
  - Additional details on later slides…

PACE objective for improving cold-start simulations

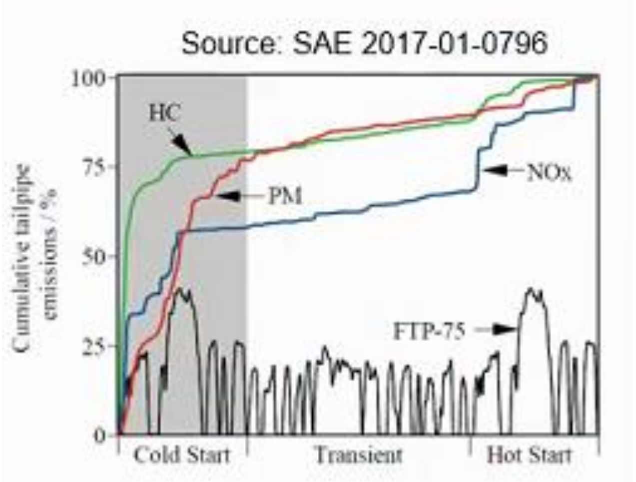
PACE consortium objectives are to…

- **Develop improved predictive simulation capabilities for key physics**
  - Spray, wall-film, ignition, kinetics, soot formation, etc.
- **Apply those improvement to key barriers to improved engine efficiency, emissions, and performance**
  - Cold-start, knock, cyclic variability, dilute operation, etc.



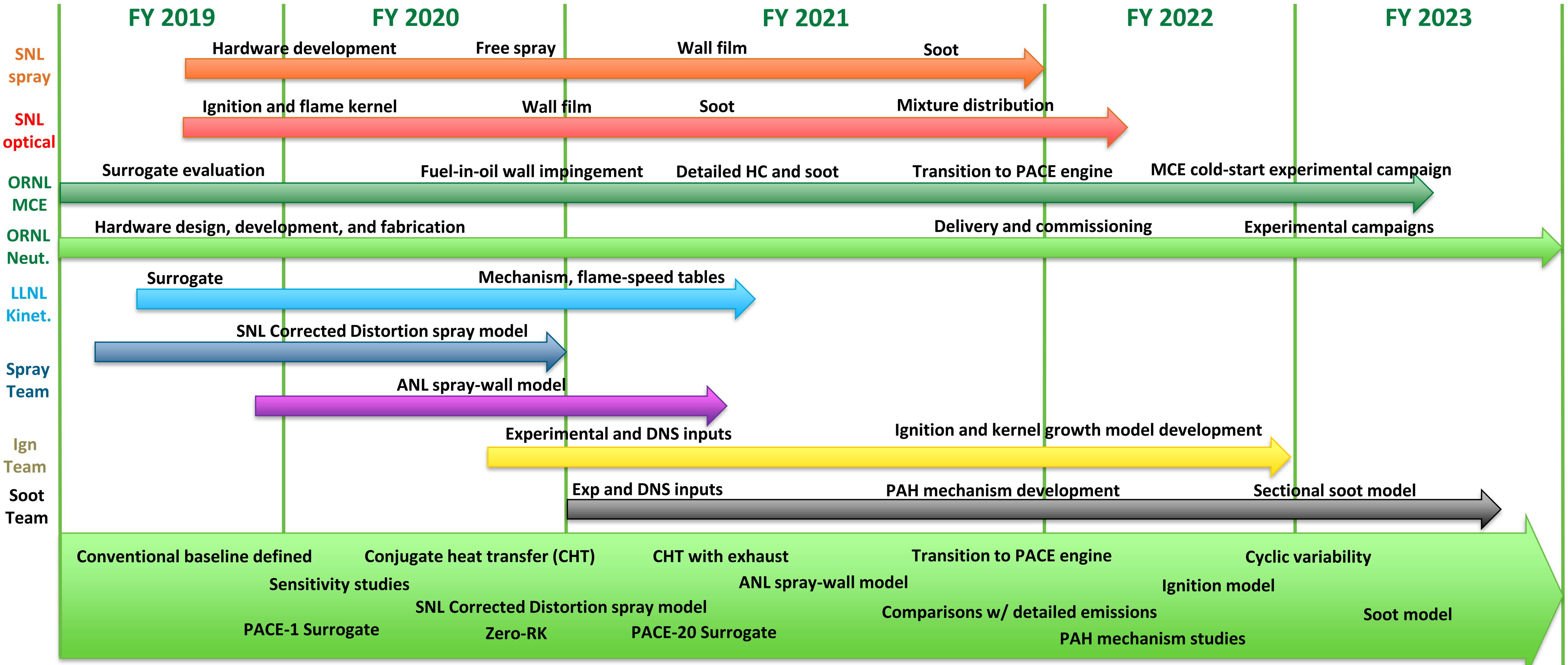
This presentation focuses on *application* of experimental learnings and new submodels to improve accuracy of cold-start simulations

- **PACE Major Objective 8**
  - *Deeper understanding of cold-start physics & chemistry to enable faster, numerically-aided design & calibration*
- **Why cold-start?**
  - Majority of EPA Federal Test Plan (FTP) emissions occur during cold-start
  - Development of operating strategies that accelerate catalyst heating would benefit from accurate simulation
  - But simulation of cold-start is very challenging with conventional methods



Timeline for selected PACE cold-start efforts

Approach

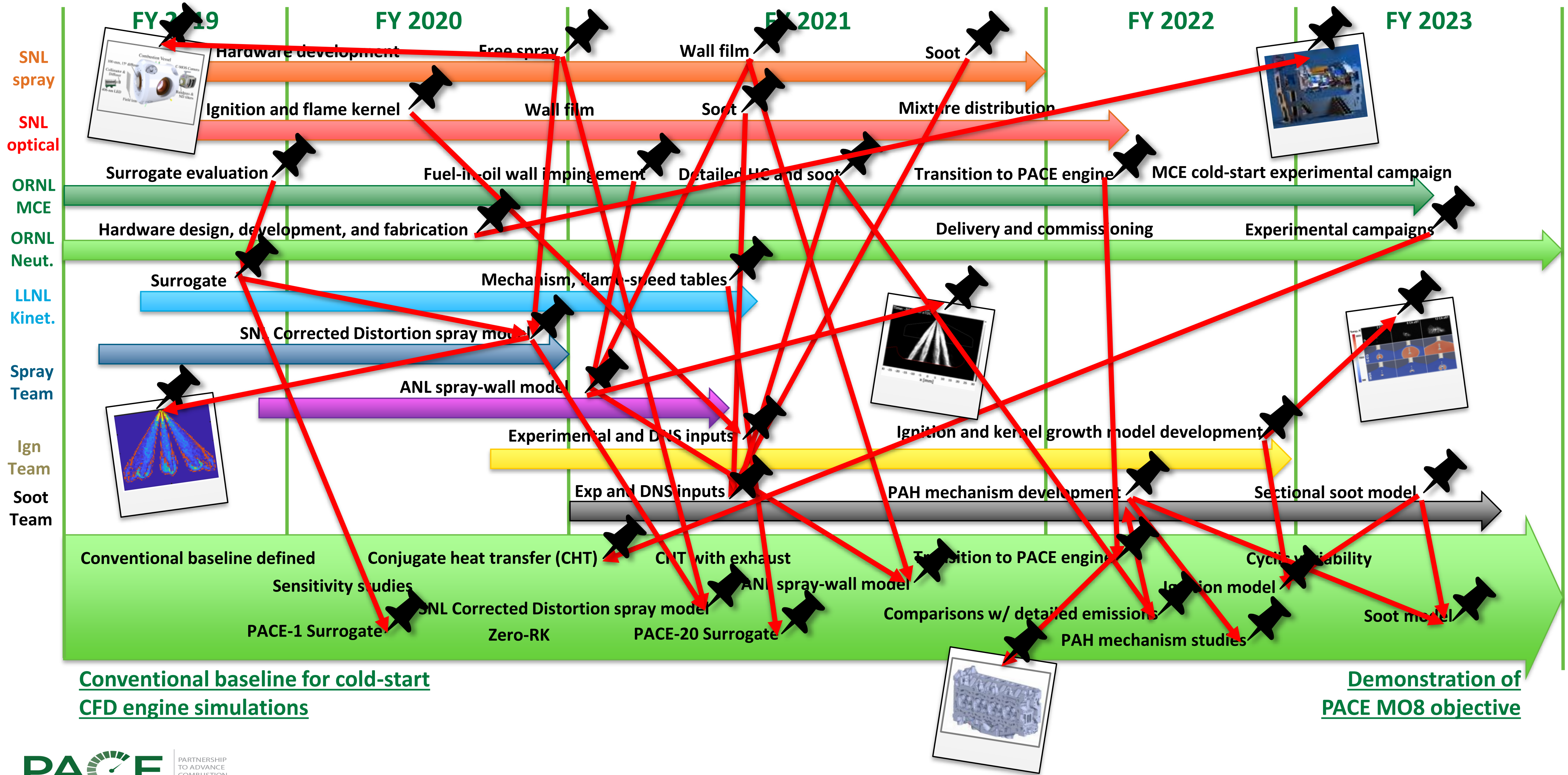


Conventional baseline for cold-start CFD engine simulations

Demonstration of PACE MO8 objective

It's all connected!

Approach



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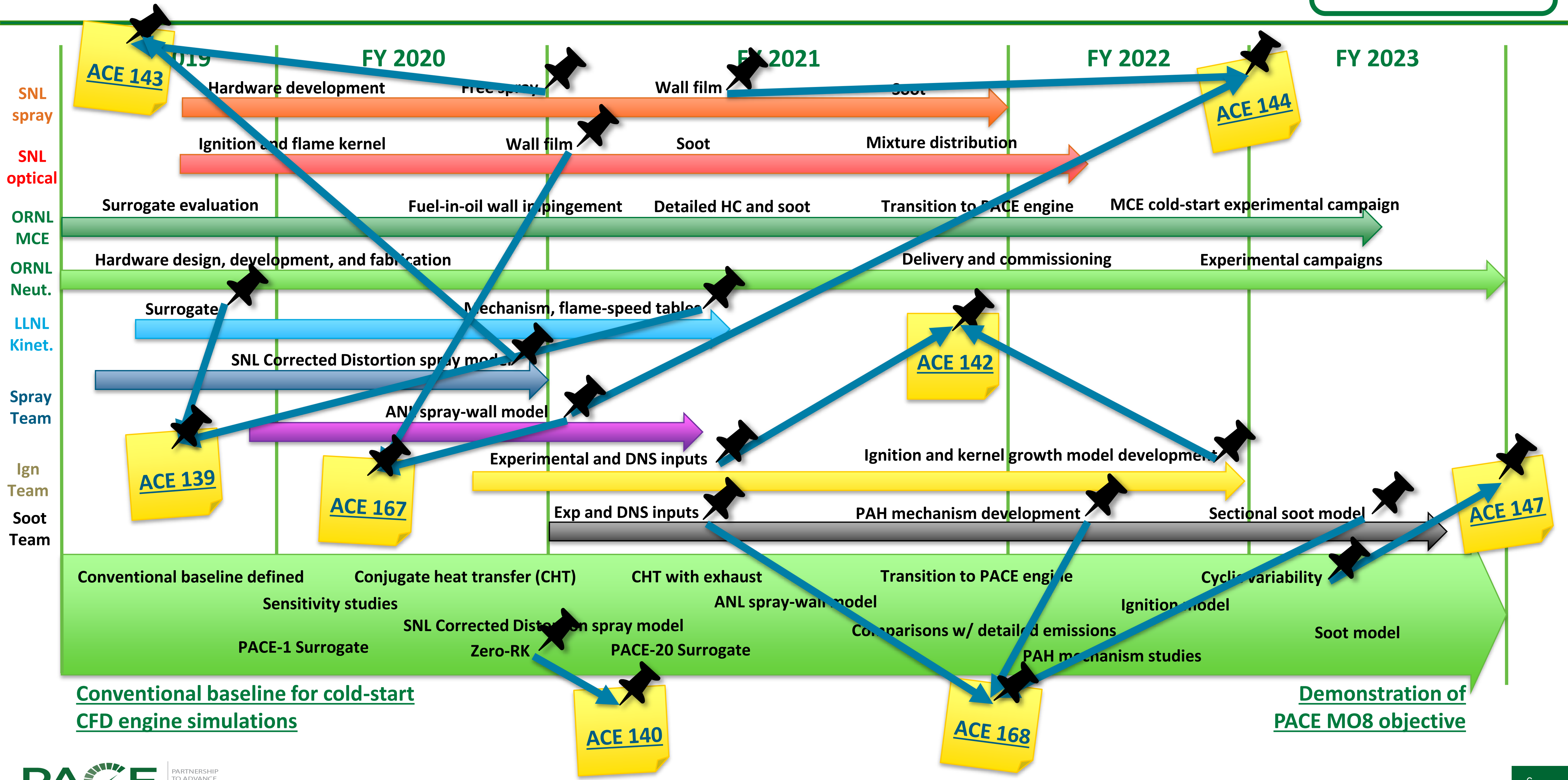

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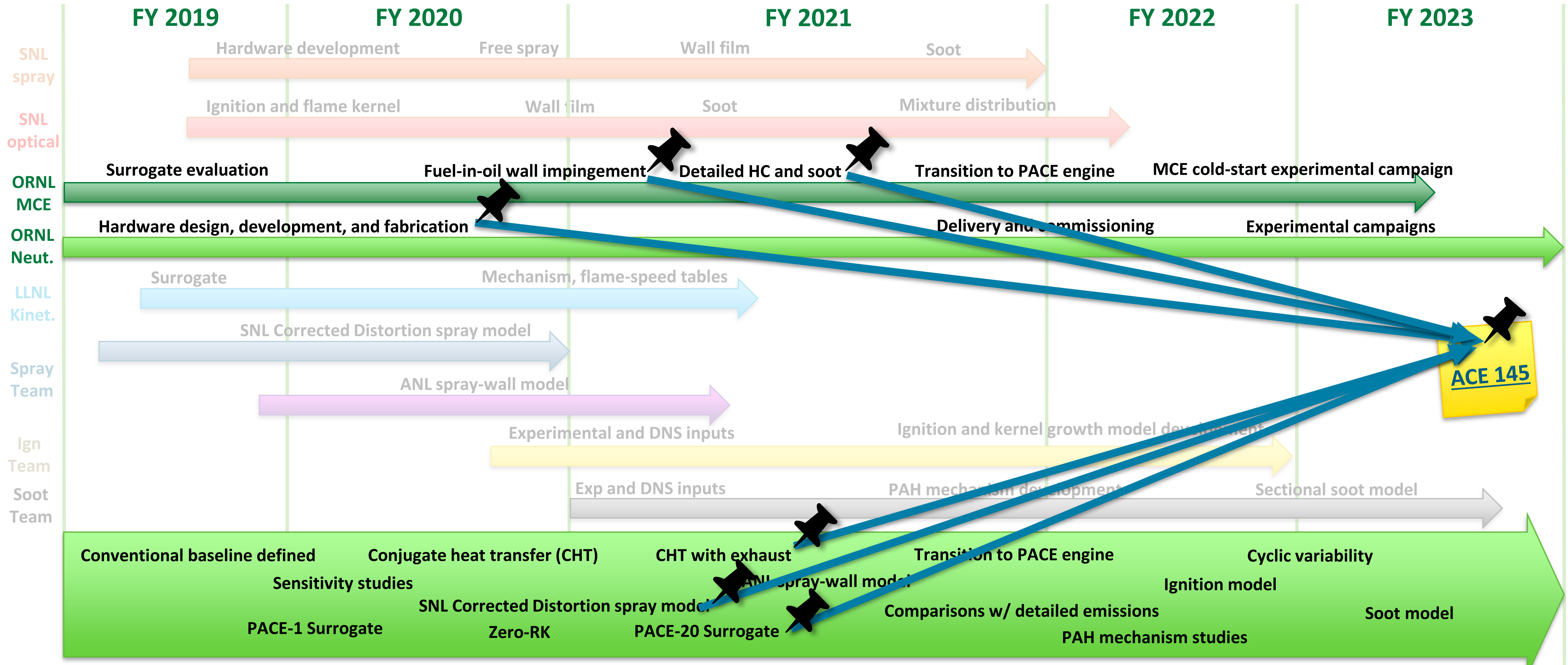


Conventional baseline for cold-start CFD engine simulations

Demonstration of PACE MO8 objective

Milestones

Date	PI	Milestone	Status
FY2020 Q3	Wissink, ORNL	Finalize design elements for engine and support systems.	**MET**
FY2020 Q4	Edwards, ORNL	Perform assessment of state-of-the-art cold-start modeling approaches to identify key gaps and needs.	**MET**
FY2021 Q1	Edwards, ORNL	Evaluate Sandia spray and evaporation model at cold-start conditions.	**MET**
FY2021 Q2	Jatana, ORNL	Quantification of fuel mass loss to the oil during the ACEC cold start protocol over a range of exhaust heat flux.	**MET**
FY2021 Q3	Edwards, ORNL	Use full-engine CFD with coupled CHT to evaluate thermal boundary conditions in engine and exhaust.	On Track
FY2021 Q4	Jatana, ORNL	Quantification of exhaust hydrocarbon species, temperature, and soot evolution over a range of exhaust heat flux.	On Track
FY2021 Q4	Wissink, ORNL	Commission neutronic engine ahead of contributing to MO3 and MO8 milestones.	On Track

Neutronic engine (PI: Wissink, ORNL)

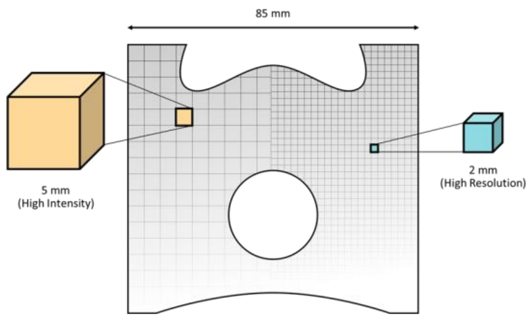
Relevance
Approach

FY 2019	FY 2020	FY 2021	FY 2022	FY 2023

Hardware design, development, and fabrication — Delivery and commissioning — Experimental campaigns

Objective

- **Obtain *in situ measurements of combustion chamber thermal boundary conditions* in a firing engine.**

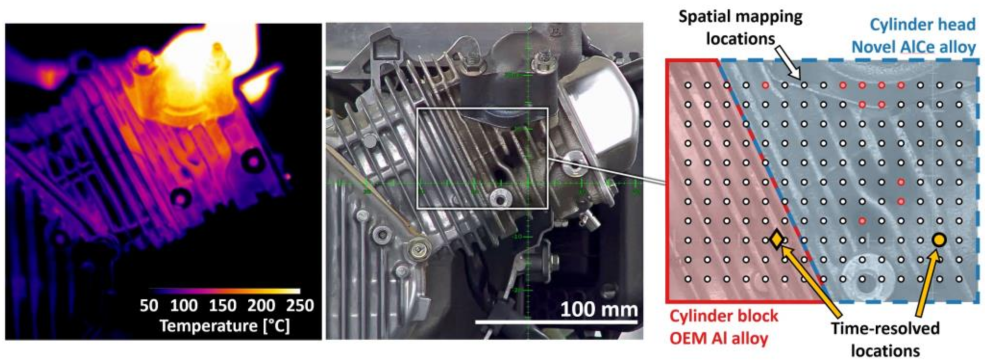


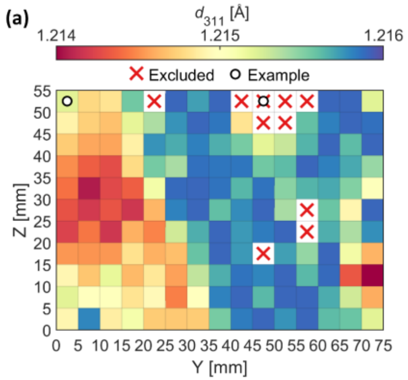
Neutron diffraction measurements made in small volume of part. Composite measurements made over full volume and through time by moving part within neutron beam.

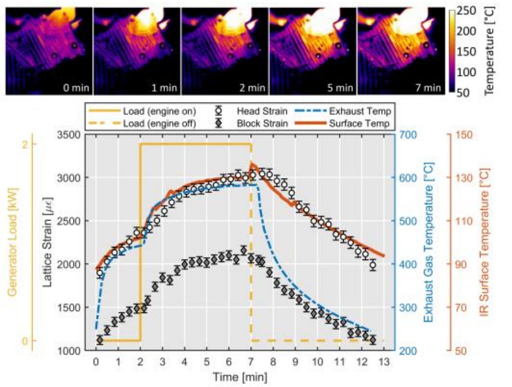
Approach

- **Neutron diffraction at ORNL's Spallation Neutron Source (SNS)**
  - Directly measures **lattice strain** inside bulk materials
  - With known material properties, provides **temperature** and **stress** throughout entire volume of part
  - Can be done under **dynamic conditions**, and even in **moving parts**
- **Developing purpose-built "neutronic engine" to enable time-resolved neutron diffraction measurements of combustion chamber thermal boundary conditions**

Real components or devices ⇨ **Spatial mapping** ⇨ **Time-resolved mapping**







Proof-of-concept was performed with small engine pre-PACE

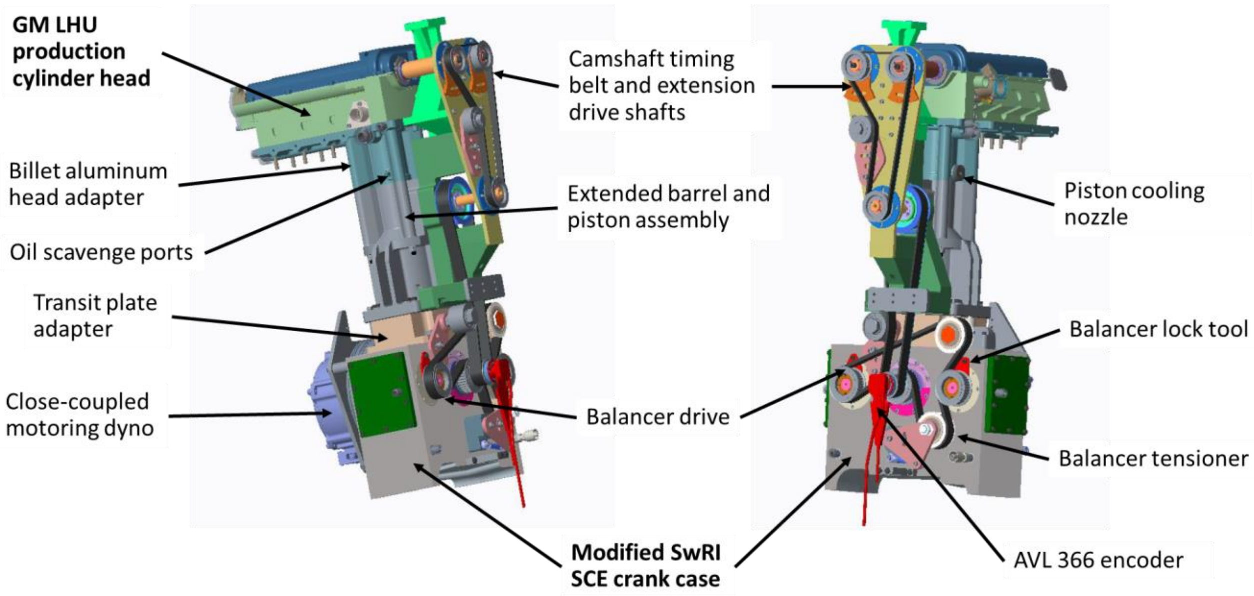
Wissink et al. (2020) Proceedings of the National Academy of Sciences, 117(52).

Neutronic Engine Design Addresses Unique Challenges

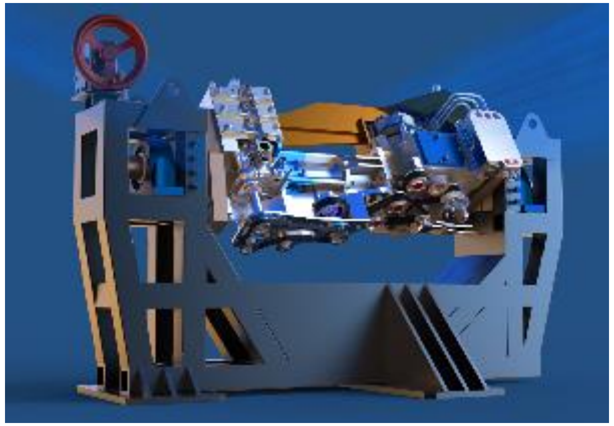
(PI: Wissink, ORNL)

- **Southwest Research Institute to design and build**
  - Subcontract issued Sept 2019
  - Midpoint design review completed Feb 2020
  - Final design review completed Sept 2020
  - Engine delivery expected July 2021
- **Engine**
  - Single-cylinder based on production GM LHU cylinder head and SwRI bottom end
  - 86-mm bore x 86-mm stroke, 4-valve, side-mount DI
  - Representative of modern SI engine, retains stock combustion chamber geometry
  - Aligns well with existing engine platforms and models at ORNL (GM LNF)
  - Fluorocarbon-based coolant and lubricant for improved neutron visibility
- **Assembly packaging**
  - Engine and close-coupled dyno mounted horizontally in rigging frame with rotational mounts
  - Fits within sample space at VULCAN instrument

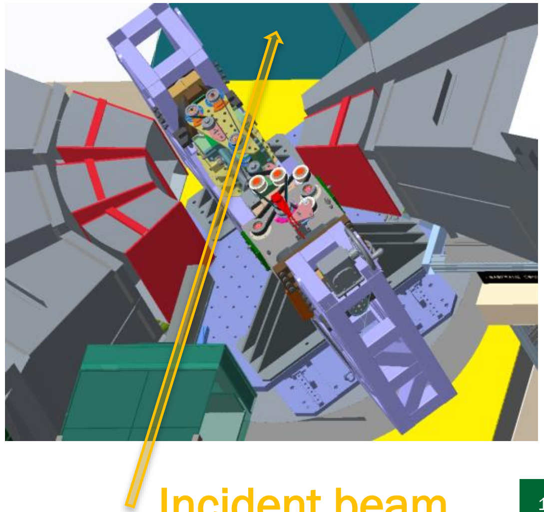
Engine design concept



Engine and frame assembly



Mounted in VULCAN diffractometer

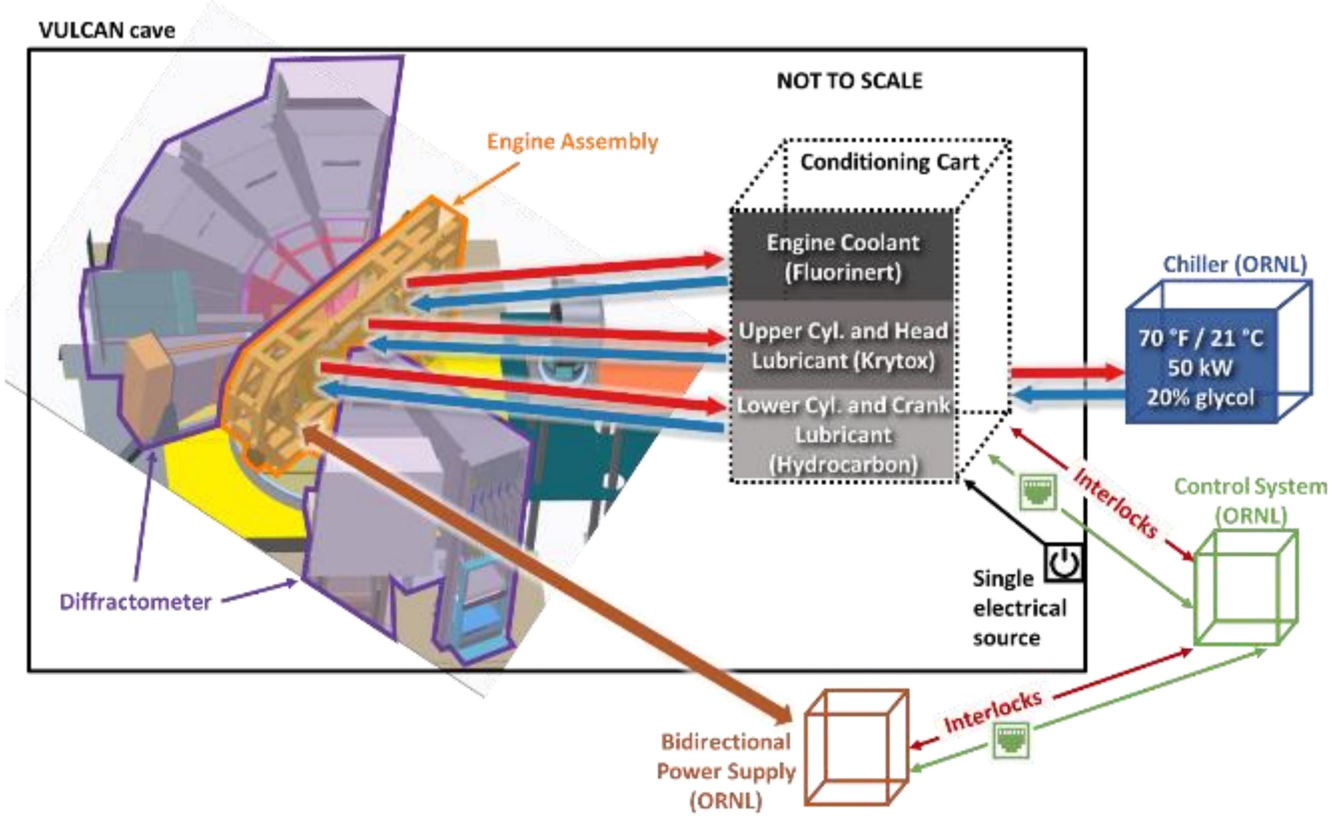


Development of facilities and support systems

(PI: Wissink, ORNL)

Tech. Accomp.
Future work

- **Highly specialized support system requirements compared to traditional single-cylinder research engines**
  - Fluorinated coolant and lubricant in certain sections of the engine
  - Multiple lubrication systems
  - Data and controls integration into a particle accelerator facility
- **Detailed Statements of Work (SoWs) prepared for coolant and lubricant conditioning system and data acquisition and controls system**
  - Conditioning system has been delivered and is undergoing commissioning
  - Subcontract has been issued for controls system with delivery expected Q3 2021
- **Facilities upgrades in progress at VULCAN**
  - Chilled glycol/water for engine cooling
  - Upgraded exhaust system to handle engine exhaust flowrate and temperature



Next steps

- **Commission engine and perform first diffraction measurements**
- **Align target operating conditions for volumetrically-resolved thermal boundary condition measurements with CHT modeling tasks**

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

Multi-cylinder cold-start testing (PI: Jatana, ORNL)

Relevance
Approach

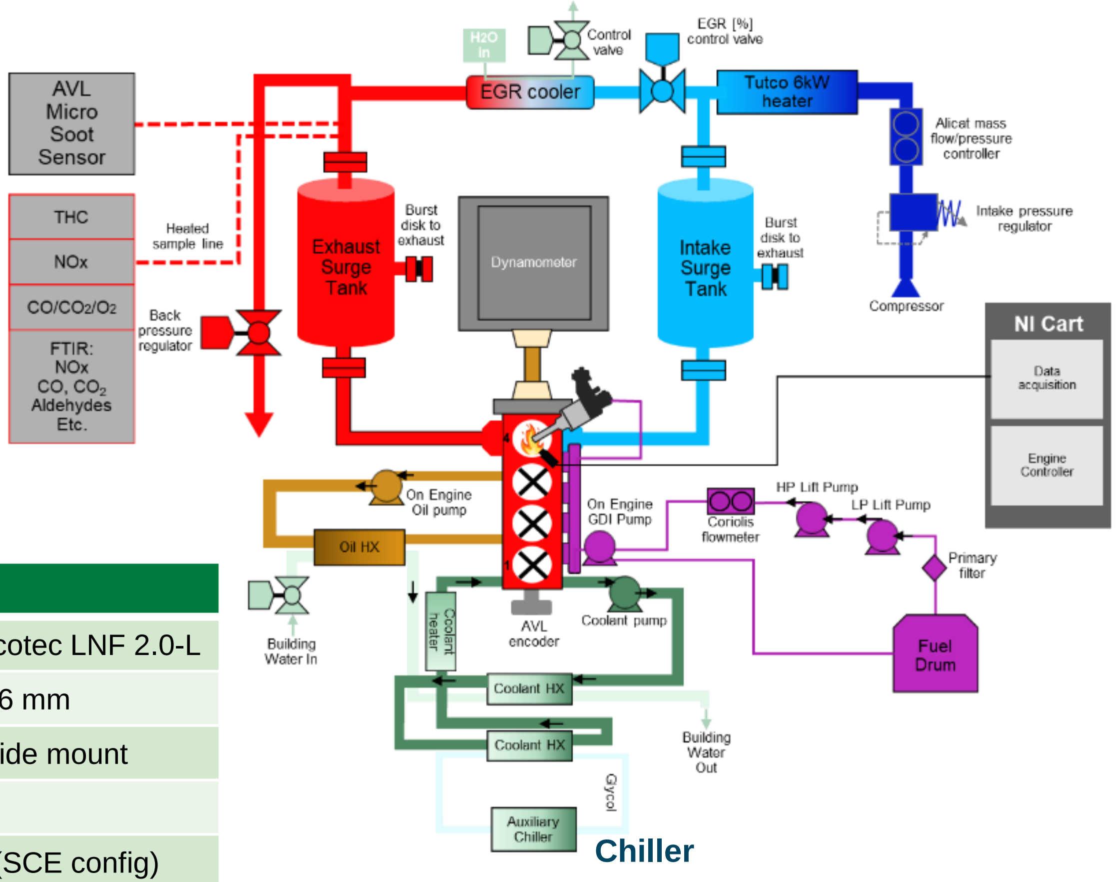
Objective

- Develop *comprehensive validation engine data* during cold-start (and warm restart) operation
  - Exhaust heat flux, emissions, thermal boundary conditions

Approach

- *Engine experiments with production hardware* converted for single-cylinder operation
  - Detailed spatial exhaust measurements and speciation
  - Intake air, outlet coolant and oil maintained at 20°C
  - ACEC Cold-Start Protocol
    - Steady-state operation
    - 1300 rpm, 2-bar NMEP
    - Sweep exhaust enthalpy
  - RD5-87 fuel

ORNL Single-Cylinder LD Platform for Cold-Start and Knock



Specifications	(-)
Base engine	GM Ecotec LNF 2.0-L
Bore x stroke:	86 x 86 mm
Injection	DI – Side mount
Base CR	9.2:1
Firing cylinder	Cyl 4 (SCE config)
SCE Displacement	500 cc

FY 2019 — Surrogate evaluation
FY 2020 — Fuel-in-oil wall impingement
FY 2021 — Detailed HC and soot
Transition to PACE engine
FY 2022 — MCE cold-start experimental campaign
FY 2023

PACE PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

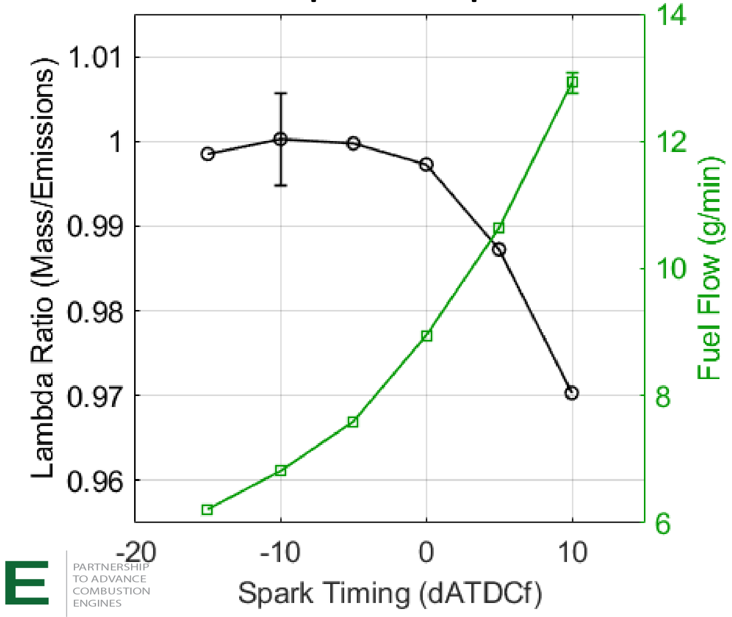
Cold-start Fuel-Loss-to-Oil Quantification (PI: Jatana, ORNL)

- **Fuel-loss-to-oil trends provide info on wall wetting for modeling**
  - Higher fuel loss at retarded spark timings – trends with increase in required fuel
    - Increase in cylinder pressure due to increased air flow also a likely factor
  - Exhaust cam retard has negligible effect on fuel loss
    - Fuel loss not trending with the higher fuel flow required at retarded exhaust cam timings
  - Start of injection (SOI) sweep
    - Likely interplay between piston and cylinder wall wetting
  - *Data is being fed into wall-wetting simulations*

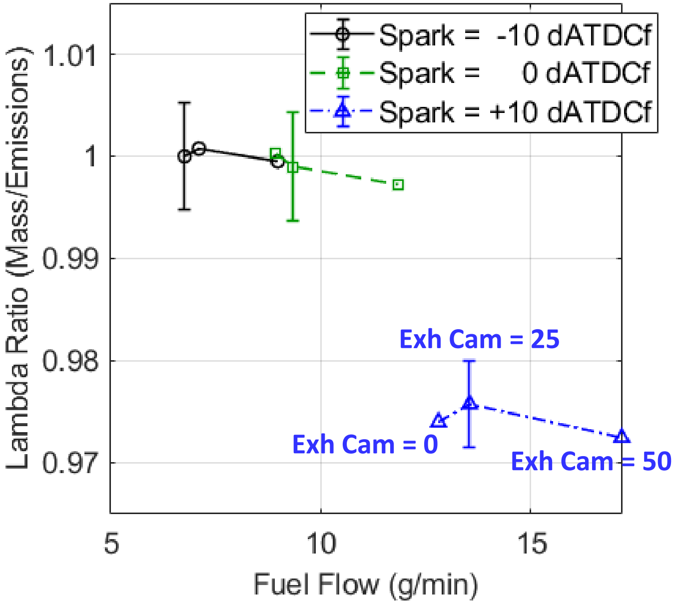
	RD5-87
Engine Conditions	**ACEC Steady-State Cold-Start Protocol**
Injection Pressure [bar]	**120**
Spark Timing [°ATDC]	**-15, -10, -5, 0, 5 and 10**
Injection Timing [°ATDC]	**Base: -280 Sweep: -290 to -230**
Lambda [-]	**1**
Cam Timings [°retard]	**Intake: 0 Exhaust: 0, 25, 50**

1300 rpm and 2-bar NIMEP stoichiometric operation

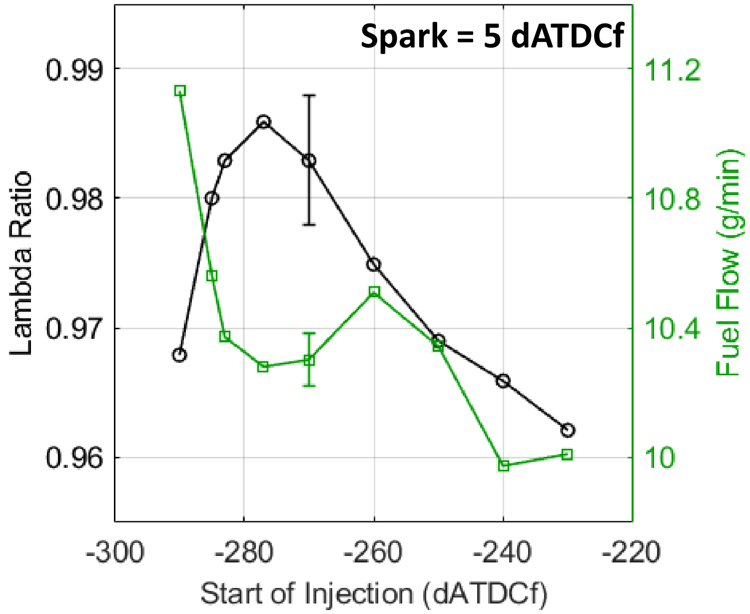
Spark Sweep



Exhaust Cam Opening Retard Sweep



SOI Sweep



Cold-Start Soot Measurements (PI: Jatana, ORNL)

- **Engine-out Soot measurements to provide model validation data**
  - Engine-out soot emissions increase with spark retard
  - Exhaust cam retard also increases soot emissions
  - Significant increase in soot emissions for very advanced injection timings
    - Likely due to piston wetting
  - *Data is being fed into wall-wetting simulations and to soot modeling team*
- **2-8kW/L exhaust heat flux range achieved with exhaust cam phasing**
  - Retarded SOI requires lower fuel flow to maintain load due to improved combustion stability

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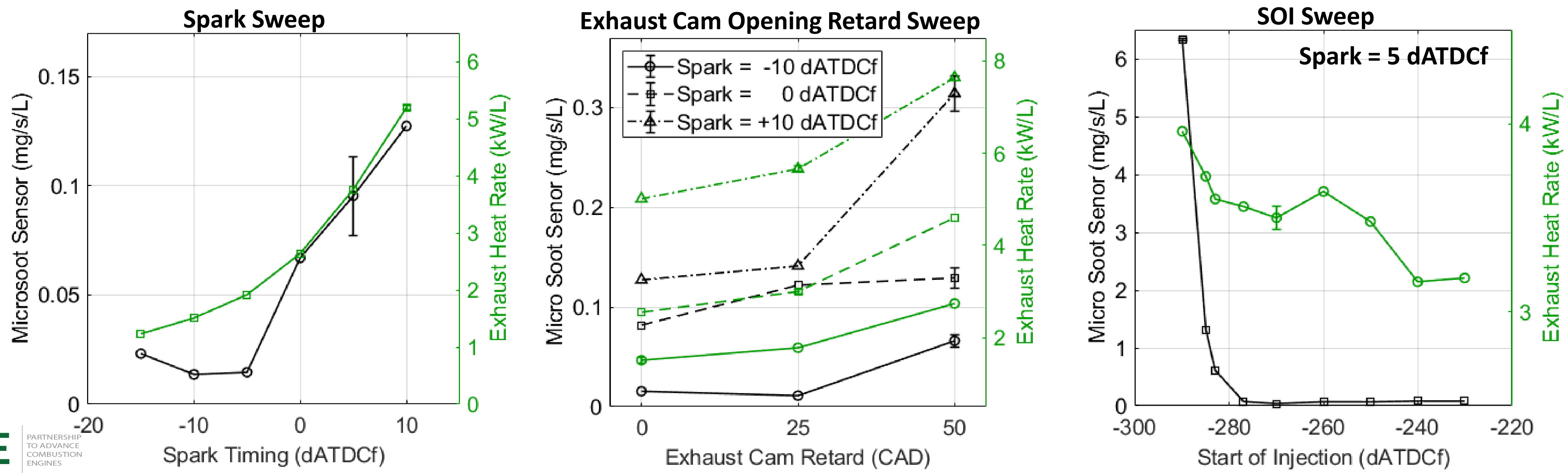

Next steps (PI: Jatana, ORNL)

Future Work

FY21 planned work

- **Complete analysis of results from recent campaign**
  - *Results will be shared with modeling teams*
- **Split injection strategies**
- **PACE-20 surrogate fuel**
- **Advanced fuel-in-oil characterization at select conditions using ORNL's laser-induced-fluorescence (LIF) measurement system**
- **Quantification and speciation of hydrocarbons and soot evolution in exhaust**
  - Cannister samples at multiple locations for HC speciation
  - Filter samples for organic/solid carbon fraction
  - PM particle size distribution with EEPS or SMPS
  - *Results will be shared with PACE soot working group*
- **Transition efforts to PACE common engine platform (Ford 2.3-L EcoBoost)**
  - Multi-cylinder production engine converted to single-cylinder operation
  - Installation underway in ORNL engine cell

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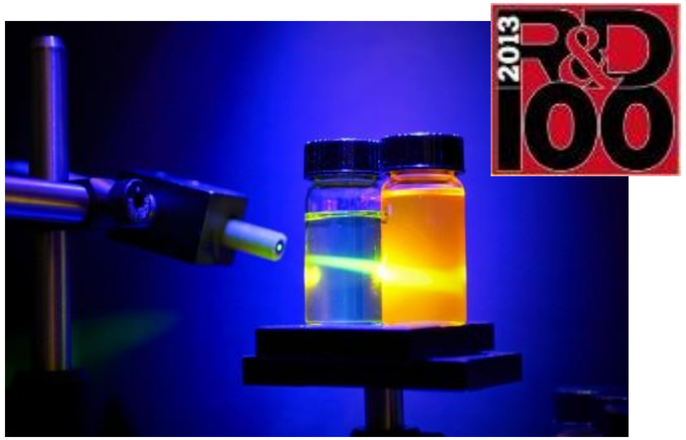
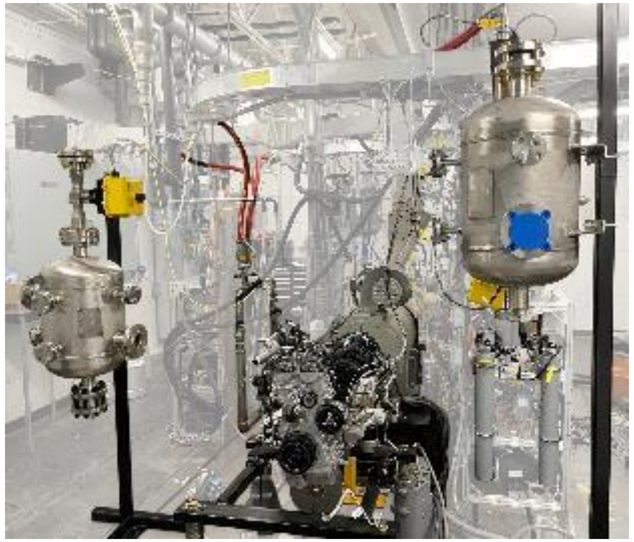
FY22 planned work

- **High-speed measurements of temperature and gas species evolution in the exhaust stream**
- **Quantification of species and temperature from engine cranking to ACEC Tech Team cold-start protocol point**

ORNL's Fuel-in-Oil LIF measurement system





Installation of the PACE common engine platform (Ford 2.3-L EcoBoost) in ORNL engine cell

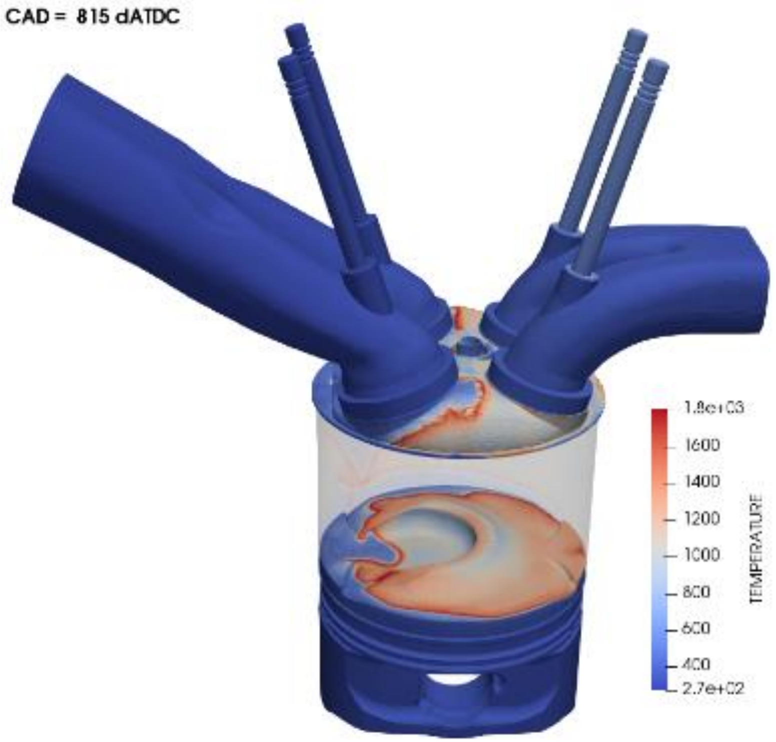
Any proposed future work is subject to change based on funding levels.

Cold-start simulation efforts (PI: Edwards, ORNL)

Relevance
Approach

Objective

- *Improved predictive simulation of cold-start* **engine operation**
  - Demonstration of PACE cold-start objective
  - Evaluate improvements to modeling of charge preparation, combustion performance, and emissions production over conventional methods



Approach

- **Apply experimental learnings and new, physics-based submodels**
  - Targeting improvements to charge preparation, ignition and combustion, and emissions generation
  - Comparison to conventional, baseline model performance
  - Validation against experimental data

FY 2019	FY 2020	FY 2021	FY 2022	FY 2023

Conventional baseline defined
Conjugate heat transfer (CHT)
CHT with exhaust
Transition to PACE engine
Cyclic variability
Sensitivity studies
ANL spray-wall model
Ignition model
SNL Corrected Distortion spray model
Comparisons w/ detailed emissions
Soot model
PACE-1 Surrogate
Zero-RK
PACE-20 Surrogate
PAH mechanism studies

Conventional baseline for cold-start CFD engine simulations

Demonstration of PACE MO8 objective

Summary of progress and accomplishments (PI: Edwards, ORNL)

Technical Accomplishments

Defined conventional baseline model and completed sensitivity studies for key submodels

- Large portion of fuel in wall film
- Highly sensitive to thermal BCs, especially evap & film
- Tw=100°C removes charge prep effects, matches well with premixed simulations
- G-equation can be tuned to match reasonably well, but not robust to changes

Results reported at 2020 Fall AEC Program Review meeting

Corrected Distortion spray model and flash boiling added

- Better evaporation of lighter components, but deeper penetration of heavier components
- Flash boiling of lighter components above 20°C at ACEC protocol conditions
- Notable changes in film formation and evolution

Results reported at 2021 Winter AEC Program Review meeting

PACE-20 surrogate added

- Included in CD spray runs
- Fired runs with CD spray and Zero-RK are in progress
- *Requiring retuning of G-eq parameters*

Will provide new benchmark for future efforts

Initial CHT cylinder runs complete

- Results show average cylinder Tw=~60°C for steady-state ACEC cold-start protocol cases

Results incorporated into future simulations

CHT runs with exhaust underway on Eagle

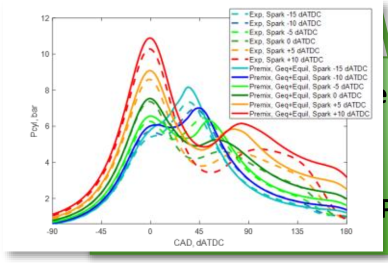
- 3-D CHT in exhaust pipe matching ORNL SCE LNF platform
- Kinetics being solved in exhaust
- Exploring sensitivity to back-side BCs

Spray-wall interaction model received

- Runs will begin once model retuned for PACE-20 surrogate

Comparison to detailed emissions

- Runs will begin once model retuned for PACE-20 surrogate



FY 2020 | **FY 2021** | **FY 2022** | **FY 2023**

e defined
Sensitivity studies
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Conventional baseline for cold-start CFD engine simulations

Demonstration of PACE MO8 objective

CD spray model and flash boiling added (PI: Edwards, ORNL)

Technical Accomplishments

Flash boiling (CONVERGE v3.0) and the Sandia Corrected Distortion spray models were added to the baseline cold-start engine model

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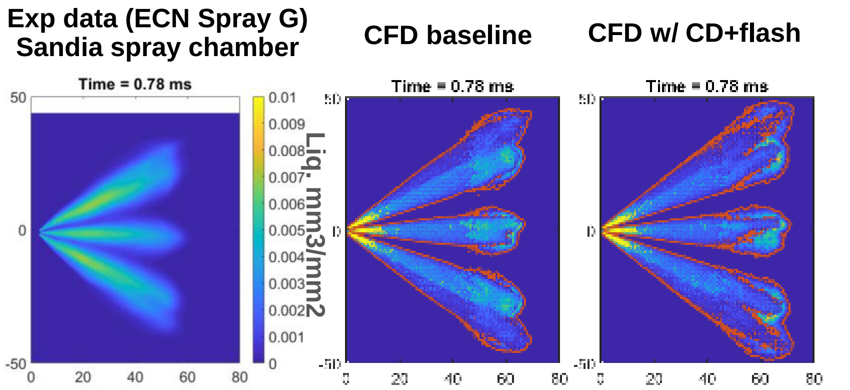
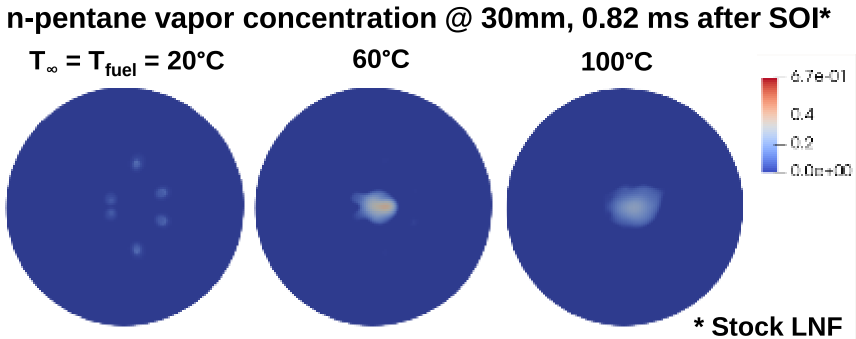
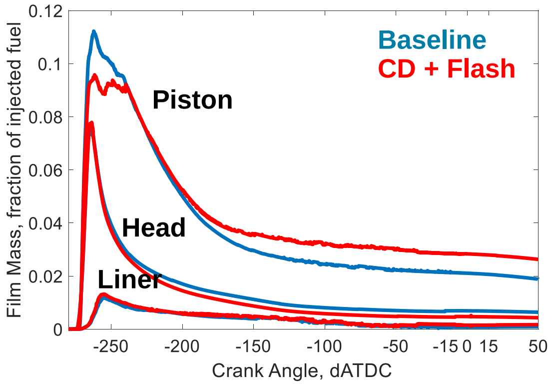
- **Free-spray and engine (GM LNF) simulations with PACE-20 surrogate**
- **Free spray (ECN Spray G) compared to experiment and baseline model**
  - CD + Flash boiling predicts better evaporation of lighter components, but deeper penetration of heavier components than baseline model
- **Flash boiling of lighter species observed at conditions above 20°C**
  - Very relevant for simulation of experiments following ACEC Tech Team cold-start protocols with steady-state operation
- **For engine, vapor composition at spark gap closer to PACE-20 definition**
  - Predicting better evaporation of most components (tetralin at 73% of PACE-20 level)
- **Notable changes in cylinder wall film with CD + Flash boiling**
  - Less initial film formation, especially on piston
  - But lower evaporation rate resulting in more film at time of spark
  - Suspected to be due to combination of…
    - changes in spray pattern due to flash boiling
    - Higher concentration of heavier species in film

Further analysis underway for future publication





* Stock LNF injector



PACE PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

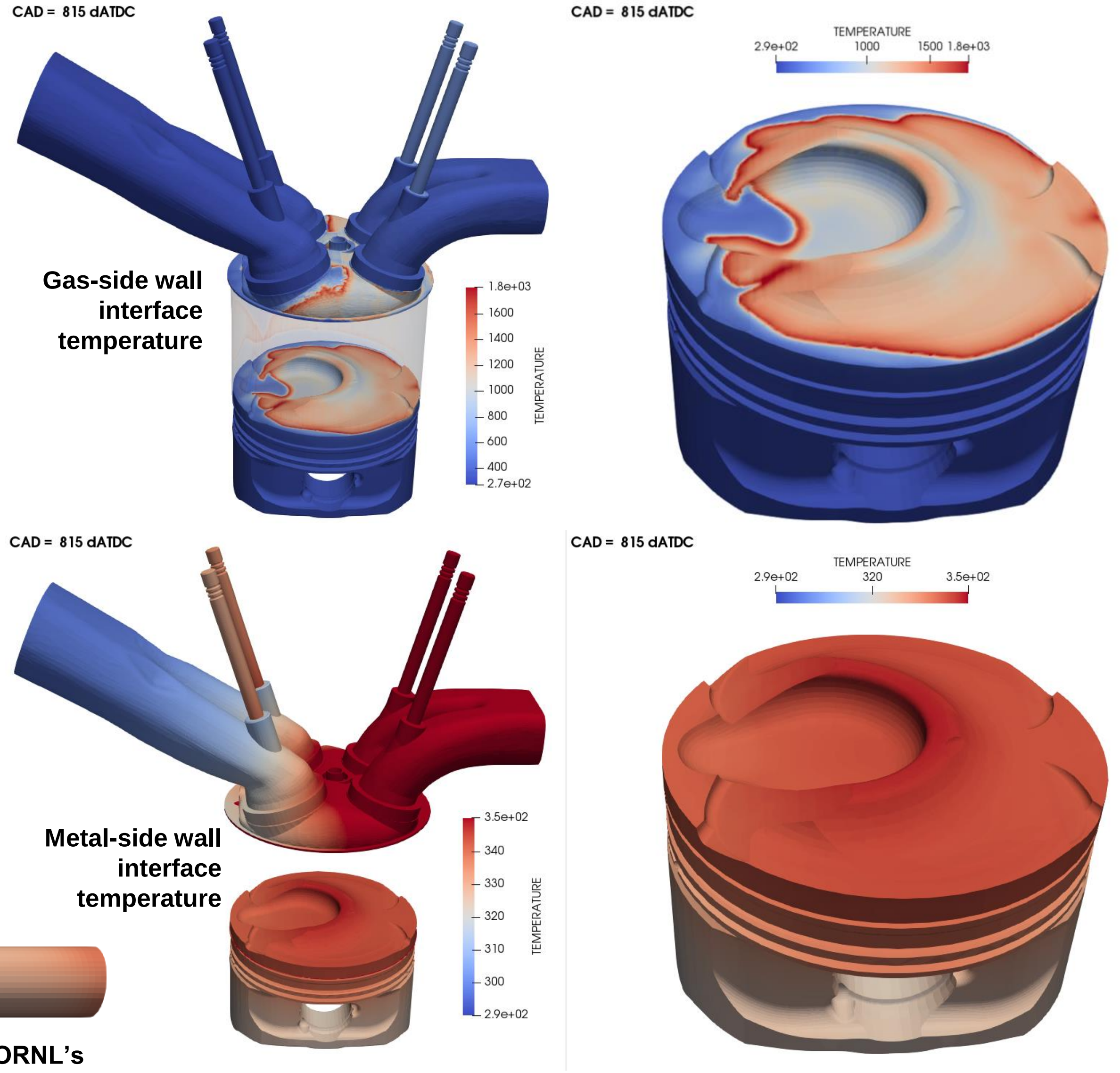
CHT simulations for improved thermal BC

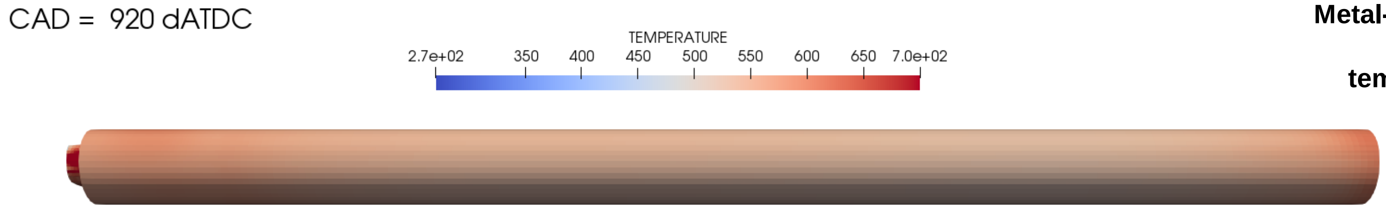
Technical Accomplishments

Coupled conjugate heat transfer (CHT) model for ORNL's modified single-cylinder GM Ecotec 2.0-L LNF engine

- **3-D CHT on piston, head, exhaust pipe; 1-D on liner**
  - GruMo-UniMORE law-of-the-wall gas-side heat transfer
  - Simulations currently being performed on Eagle
- **Predicted spatio-temporal average cylinder wall temperature ~60°C**
  - Significant spatial variability (~40°C) in head temperatures for steady-state operation under ACEC cold-start protocol
  - Temporal variability is limited with minor increases during combustion
- **Examining sensitivity to back-side BCs**
  - Initial results converging suggesting limited sensitivity
- **Exhaust geometry used on SCE for exhaust sampling**
  - Spatial variation of ~50°C along length
- **More detailed analysis pending completion of runs**

CHT surface temperature predictions during combustion





38-in exhaust pipe used for detailed exhaust sampling on ORNL's modified single-cylinder GM Ecotec 2.0-L LNF engine

Next steps (PI: Edwards, ORNL)

Future Work

FY21 planned work

- **Complete CHT runs with exhaust system for BCs and emissions**
  - *Results will be shared with modeling teams*
- **Comparison to detailed emissions and soot measurements (PI: Jatana, ORNL)**
  - Comparisons for CHT runs w/exhaust (PACE-1/8 surrogate) and cyl model (PACE-20)
- **Add Argonne NL Spray-Wall Interaction model (PI: Torelli, ANL)**
  - Coupling with Sandia Corrected Dispersion spray model already established
  - Has already shown significant improvement in film predictions for SNL optical engine
  - *Model has been delivered, awaiting retuning of model with PACE-20 surrogate*
- **Begin transition to modeling PACE common engine (Ford 2.3-L EcoBoost)**
  - Geometry model being reconstructed from CT and laser scans of production hardware
    - Collaboration with LaserDesign and Convergent Science
  - Injector characterization in planning

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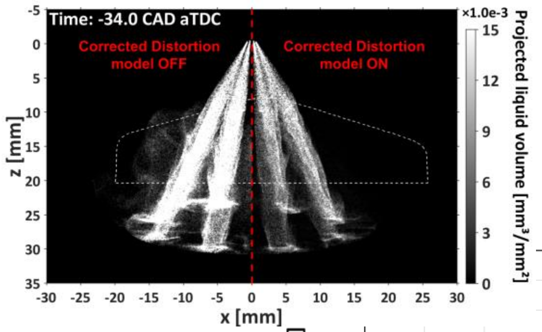
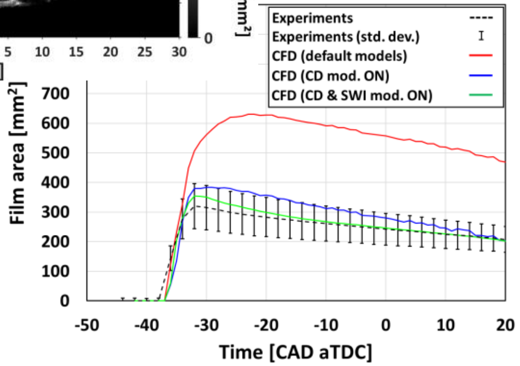
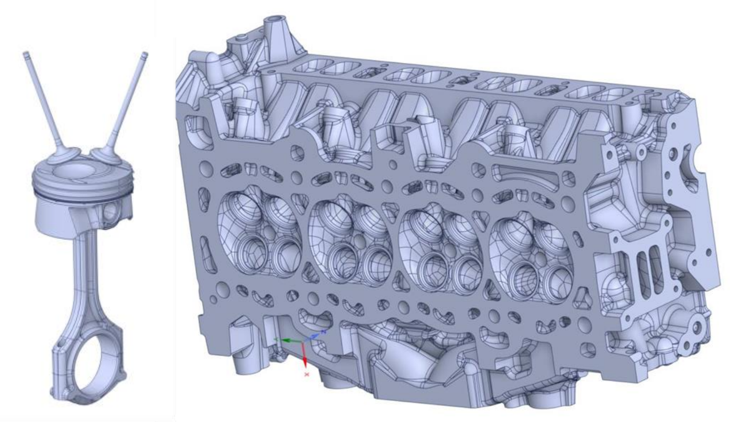




Improved film prediction with coupled CD and SWI models over conventional models (Credit: Argonne NL)



Geometry reconstruction of common PACE engine platform production hardware (Ford 2.3-L EcoBoost) from CT and laser scans by LaserDesign, Inc.

FY22 planned work

- **Commission and validate PACE engine model with experimental data**
- **Add ignition and quenching models (PI: Scarcelli, ANL)**
- **PAH mechanism studies (PI: Kukkadapu, LLNL)**

ACE 142

ACE 168

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

Remaining challenges and barriers

Overall challenges and barriers for PACE program are covered in ACE 138

- **Neutronic engine (PI: Wissink, ORNL)**
  - Management of neutronic engine design, build, and commissioning
  - Integration of neutronic engine and specialized support systems into the VULCAN beamline
  - Development of techniques for spatiotemporal alignment and binning of engine and diffractometer data to enable time-resolved measurements in moving parts
- **Multi-cylinder cold-start testing (PI: Jatana, ORNL)**
  - Provide critical data sets for model validation including quantification of exhaust hydrocarbon species, temperature, and soot evolution over a range of exhaust heat flux
  - Transition approach to PACE engine from current work on GM LNF
- **Cold-start simulation efforts (PI: Edwards, ORNL)**
  - Integration of various submodels into CONVERGE and evaluating any potential unintended interactions
  - Accurate prediction of emissions is challenging even under normal operation

Responses to previous reviewer comments

Neutronic engine (PI: Wissink, ORNL)

- ***"How much can be acquired. Is it an ensemble averaging process in both x, y, z and time? How many unique conditions can be measured considering the complexity?"***
  - *<u>ORNL response:</u> The diffraction data is ensemble averaged over position (x,y,z), and time. The number of conditions possible would depend on the size of the volumetric region that needs to be resolved as well as the temporal resolution (cycle average vs. crank angle resolved). Mapping the full combustion chamber at high time resolution for a single condition could take several days but measuring a single location's cycle-average could be done in minutes.*

Multi-cylinder cold-start testing (PI: Jatana, ORNL)

- ***"Consider adding a higher speed/load condition to the work."***
  - *<u>Engine experiment response (SNL + ORNL + ANL):</u> This is very helpful feedback. Adding a higher load point for an engine thermal state that corresponds to 20 s into the cold-start is something that we would be interesting in pursuing if time and resources allow. The future work plan includes investigating transient aspects of cold-start.*
- ***"… it is not certain if soot modeling can be accurate for a wide range of cold-start operation as the current surrogate fuel showed a big difference with the reference fuel RD5-87 in higher exhaust heat flux range."***
  - *<u>ORNL response</u>: The initial experiments gave valuable feedback on surrogate performance, an important part of the collaborative nature of PACE. A new surrogate (PACE-20) has now been developed which includes tetralin to better match the high end of the boiling curve.*
- ***"Can this engine be used to study the effect of injection and spark parameters on engine performance during the ACEC Cold start test?"***
  - *<u>ORNL response</u>: The future workplan includes investigation of multiple injections and spark parameters including heat range of the spark plugs.*

Cold-start simulation efforts (PI: Edwards, ORNL)

- ***"[Need to] understand where the discrepancies in modeling are arising from… every aspect of the model should be introspected and compared with fundamental experiments with cold walls."***
  - *ORNL response: This is the approach being taken under PACE with teams looking at each aspect of charge preparation, ignition and combustion, and emissions both experimentally and in models. This task takes those learnings and applies them to evaluate resulting impact on cold-start prediction.*

Collaborations and Acknowledgements

PACE is a DOE-funded consortium of 5 National Labs collaboratively working toward common objectives

Overall PACE objectives and work plan were developed with input from key stakeholders including DOE, U.S. DRIVE ACEC Tech Team, and Advanced Engine Combustion (AEC) MOU members including CFD software vendors.

- **Neutronic Engine (PI: Wissink, ORNL)**
  - Subcontract with SwRI to design and build neutronic engine
  - Internal collaboration with ORNL Neutron Sciences Directorate to develop facilities, sample environment, and data reduction approaches
- **Multi-cylinder cold-start testing (PI: Jatana, ORNL)**
  - Validation data provided to modeling teams
- **Cold-start simulation efforts (PI: Edwards, ORNL)**
  - Convergent Science: Licenses, support and assistance with development of CHT and PACE engine models
  - ORNL: Experimental validation data from LNF engine
  - LLNL: PACE RD5-87 surrogate kinetic mechanism and flame-speed tables
  - LLNL: Zero-RK
  - PACE Spray Team:
    - Free-spray experimental data (Pickett, SNL)
    - Corrected Distortion spray model (Nguyen, SNL)
    - Spray-Wall Interaction model (Torelli, ANL)
  - PACE Ignition Team: Ignition model (Scarcelli, ANL)
  - PACE Soot Modeling Team: Data exchange, PAH mechanism testing

Portions of this research used resources of the Compute and Data Environment for Science (CADES) at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

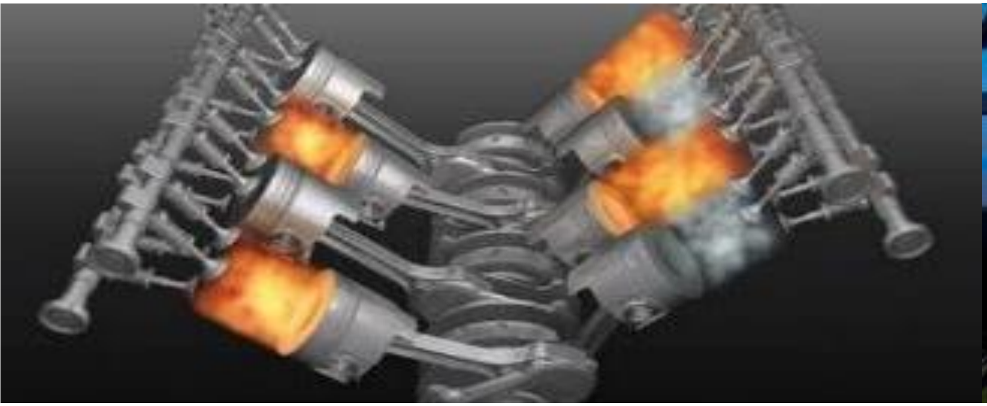
Portions of this research were performed using computational resources (Eagle) sponsored by the Department of Energy's Office of Energy Efficiency and Renewable Energy and located at the National Renewable Energy Laboratory.

Summary

Overall summary of PACE consortium objectives and work plan provided in ACE 138

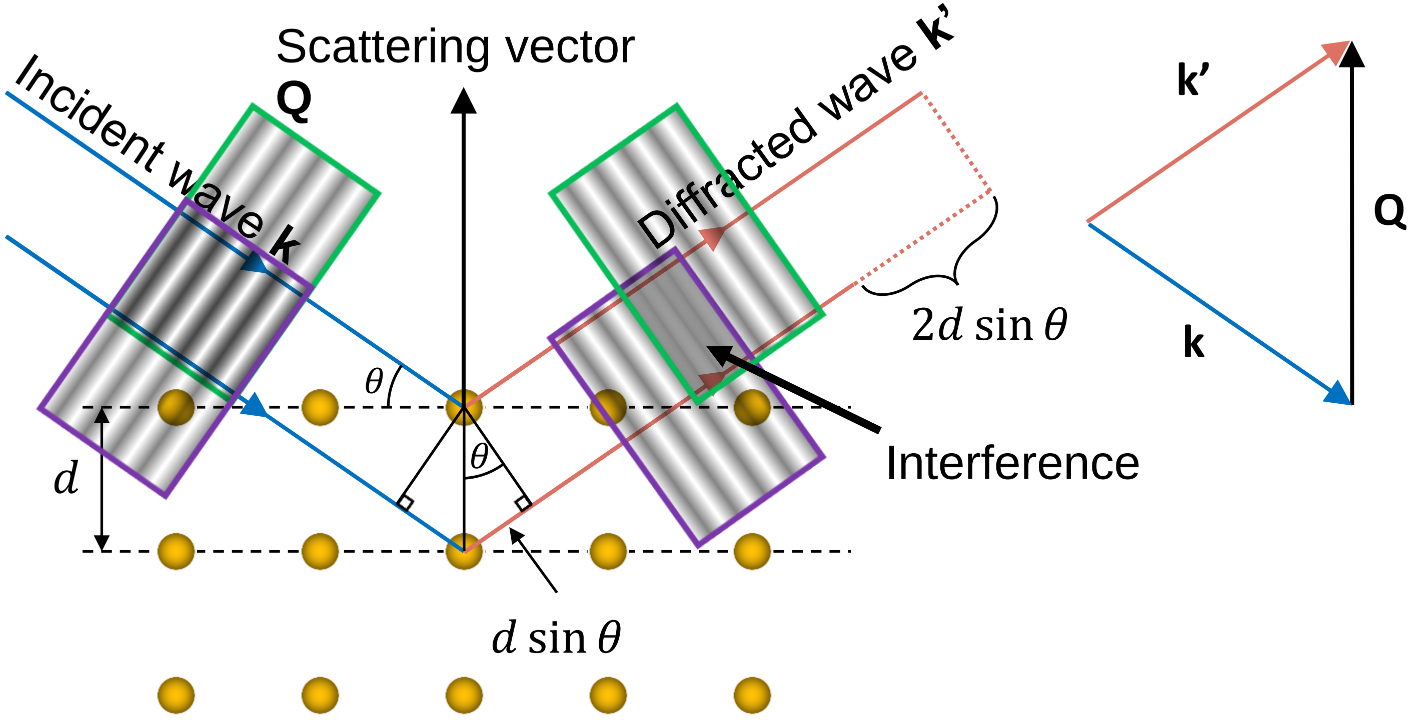
- **Relevance**
  - Addresses need for improved simulation of cold-start operation identified in U.S. DRIVE Roadmap and PACE objectives
- **Approach**
  - Experiments to provide understanding and validation data that feeds development of improved submodels and full-engine CFD
- **Technical Accomplishments**
  - Completed final design review for neutronic engine with delivery expected summer 2021
  - Completed fuel-loss-to-oil quantification and exhaust and soot measurements from single-cylinder GM LNF engine
    - Achieved 2-8 kW/L exhaust enthalpy with retarded spark timing and EV phasing
  - Added Corrected Distortion spray model, flash boiling model, and PACE-20 surrogate chemistry to baseline model
    - Provides next performance benchmark toward demonstration of PACE cold-start objective
- **Collaborations**
  - Strong collaboration between multiple NLs with guidance and support from industry
- **Future Work (Any proposed future work is subject to change based on funding levels)**
  - Commission neutronic engine and perform initial experiments
  - Detailed exhaust and soot measurements at multiple locations in exhaust system
  - Continue to add new PACE submodels including spray-wall interaction and ignition models
  - Transition efforts to the PACE common engine platform (Ford 2.3-L EcoBoost)

Technical Backup Slides



Measuring strain with neutron diffraction

- **Bragg's Law defines the condition for constructive interference when a wave is diffracted by a repeating crystal lattice**
- **The angle θ at which we measure the intensity of the diffracted neutrons is defined by the geometry and orientation of the detectors and collimators**
- **The wavelength λ of the diffracted neutrons is calculated by measuring the time of flight of the pulsed neutrons**
- **With the θ and λ we can correlate intensity peaks in the diffraction signal to interplanar spacing *d***
- **Spatial or temporal variations in d-spacing provide a direct measure of lattice strain within a given gauge volume at resolution <100 microstrain**



Bragg's Law: $2d\sin\theta = n\lambda$

Lattice strain: $\varepsilon = \dfrac{d - d_0}{d_0}$

ACEC Protocol

ACEC Protocol ANL/ORNL/SNL*

Approach:	TWC
Mode:	catalyst heating
Engine speed	**1300 rpm**
NMEP	**200 kPa**
Coolant temperature (coolant out of engine) Intake air temperature (ambient)	**20 °C**
[1,2]Heat flux	**sweep from 3 to 10 kW/L**
Lambda	**1.00**

Table from Chauhy AEC presentation Feb 2020

Targets

Approach:	LDV/LDT TWC	(-)
Mode:	catalyst heating	
Feedgas NMHC+NOx	<17 (4.8)	g/hr/liter (mg/s/liter)
Feedgas CO	<350 (97)	g/hr/liter (mg/s/liter)
PM	<1.0 (0.3)	g/hr/liter (mg/s/liter)
[1]Exhaust temperature	**> 450**	**°C**
[2]Combustion stability	<0.45	bar
COV IMEP	**<20**	**percent**

PACE PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

ORNL Experiments conducted in stock LNF engine configuration

- Stock engine configuration for SCE.
- Fuels are compared under catalyst heating mode defined by USDRIVE ACEC Tech Team.
- Spark timing is swept from -15°ATDCf to +10°ATDCf to cover exhaust enthalpy space.
- Exhaust cam timing phasing
  - 0, 25, and 50 CAD retard
  - 0 = maximum NVO
- Injection timing sweep
  - -290 to -230 dATDCf

GM LNF	Value
Bore x Stroke [mm]	86 x 86
Conrod Length [mm]	145.5
Wrist pin offset [mm]	0.8
Compression Ratio [-]	Stock (9.2)
Fuel Injection System	Direct Injection, side-mounted, production injector

	RD5-87
Engine Speed [rpm]	1300
Coolant, Oil and Air Intake Temperature [°C]	20
Load [NIMEP]	2
Injection Pressure [bar]	120
Spark Timing [°ATDCf]	15, 10, 5, 0, -5 and -10
Injection Timing [°ATDCf]	Base: -280 Sweep: -290 to -230
Lambda [-]	1
Cam Timings [°retard]	Intake: 0 Exhaust: 0, 25, 50

Exhaust Cam Phasing (PI: Jatana, ORNL)

- **Exhaust cam opening retard significantly impacts cold start performance**
  - Sharp increase in COV at highly retarded phasing
  - Increase in exhaust temperature, exhaust heat rate, and % of fuel energy present in the exhaust stream.
  - Emissions reduction observed

Able to achieve exhaust enthalpy up to 8 kW/L by varying both spark timing and EVO