PARTNERSHIP
TO ADVANCE
COMBUSTION
ENGINES

Cold-start physics and chemistry in combustion systems for emissions reduction

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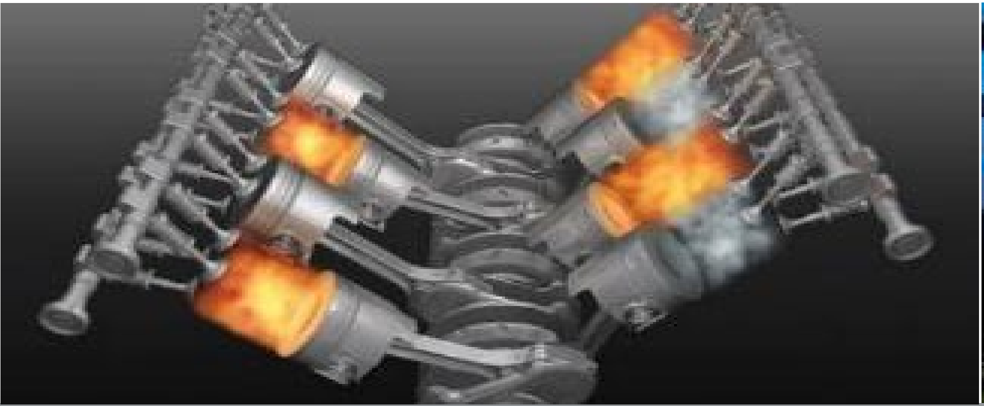
Project ID: ACE149

DOE VTO AMR, June 2020



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.

ACE149 Overview: PACE Cold-Start Modeling for Emissions Reduction

Timeline [a]

- PACE Started in Q3, FY19
- PACE will end in current form in FY23 (~25% complete)
- Focus and objectives of tasks will be adjusted
- Overall PACE work plan discussed in **ACE 138**

Budget

Task	FY19	FY20
A.01.03 (Pitz) PAH Kinetics		$200k
E.01.02 (Sjöberg) Single-cylinder DISI CS Scoping	$135k [b]	$270k [b]
F.01.01 (Rockstroh) Pre-chamber cold start		$180k [c]
E.01.01 (Curran) Multi-cyl CS & surrogate testing	$125k	$350k

a. Start and end dates refer to the life cycle of the PACE Combustion Consortium
b. Results and identical budget numbers also reported in ACE144.
c. Split results – also shown in ACE 141
d. Goals and Barriers from 2018 ACEC TT Roadmap
- https://www.energy.gov/sites/prod/files/2018/03/f49/ACEC_TT_Roadmap_2018.pdf

Barriers [d]

- **US DRIVE Priority 1:**
  - **Reduced cold start emissions**
  - Understand and improve dilute combustion strategies during cold start & cold operation to reduce emissions
  - Understanding and robust modeling tools for rapidly screening proposed designs based on sound metrics are lacking
- **PACE Outcome 8:** Validated cold-start modeling capability

Partners

- **PACE is a DOE-funded consortium of 6 National Laboratories working towards objectives ACE 138**
  - Goals and work plan developed considering input from stakeholders including DOE, ACEC Tech Team, CFD code developers, and more
- **Specific partners on the work shown here:**
  - Industry partners in AEC MOU
  - LLNL on surrogate development and kinetics
  - Modeling tasks across different teams
  - Interactions on 8 outcomes
  - *+ Many more – details in later slides*

Relevance: PACE Purpose/Objective and ACEC Barriers

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PACE Purposes in ACE 138

Emission Reduction Purpose Outcome 8

Goals and Barriers from 2018 ACEC TT Roadmap*

*www.energy.gov/sites/prod/files/2018/03/f49/ACEC_TT_Roadmap_2018.pdf

Overall Relevance of PACE:

PACE combines unique experiments with world-class DOE computing and machine learning expertise to speed discovery of knowledge, improve engine design tools, and enable market-competitive powertrain solutions with potential for best-in-class lifecycle emissions

The PURPOSES enable the OEMs to use new simulation tools and knowledge to make an engine performance breakthrough

Presentation Specific Relevance: Outcome 8 supporting PACE purpose

Purpose: Deeper understanding of cold-start physics to achieve faster, numerically-aided calibration

Outcome 8: Validated cold-start modeling capability that accurately predicts injection and spark timing trends on combustion phasing and emissions at catalyst warm-up conditions

Presentation Specific Relevance: US DRIVE – ACEC Priority 1:

- **Reduced cold start emissions**
- Understand and improve dilute combustion strategies during **cold start & cold operation** to reduce emissions
- Understanding and **robust modeling tools** for rapidly screening proposed designs based on sound metrics are lacking

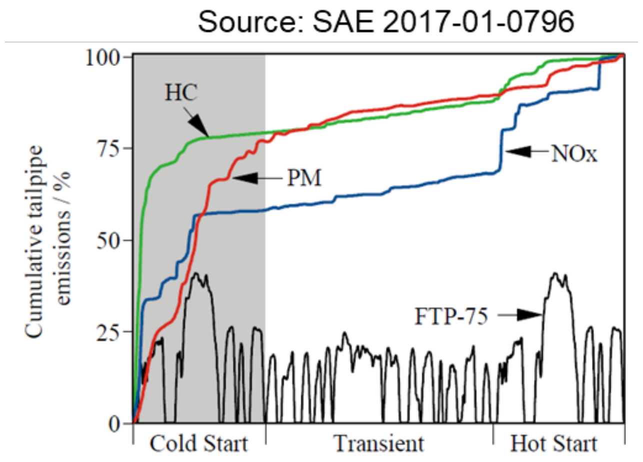
Milestones: Met or On Track

Month/Year	Description of Milestone		Status
Q3/2019	E.01.02. New AVL Micro Soot Sensor and AVL Advanced Particle Counter fully commissioned in Sandia Alt. Fuels DISI Engine Lab	SNL	Complete
Q1/2020	A.01.02a. Identify optimal reduced kinetic surrogate mechanism for DNS/LES simulations of cold-start ignition. LLNL status "completed"	LLNL	Completed
Q3/2020	A.01.03. Improved model for PAH and soot predictions validated against PAH and soot measurements in premixed and counter-flow diffusion flames for neat fuels and TPRF (toluene, n-heptane & iso-octane). Also validated against soot measurements in combustion spray chamber for gasoline fuel(s).	LLNL	On Track
Q3/2020	E.01.01. Compile large datasets of cycle-resolved combustion data for at ACEC cold start protocol conditions.	ORNL	On Track
Q4/2020	F.01.01. Experimental quantification to address the cold-start barriers of an active pre-chamber ignition system	ANL	On Track
Q4/2020	E.01.01. Exhaust hydrocarbon speciation for range of heat-flux conditions with matching in-cylinder.	ORNL	On Track

Technical Approach: Deeper understanding of cold-start physics to achieve faster, numerically-aided calibration | Collaboration on data sets to improve models

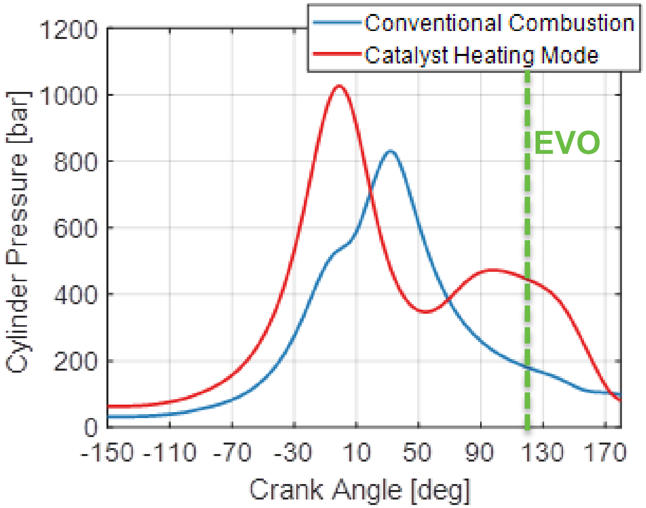
PACE Major Outcome 8: Enable zero-impact tailpipe emissions aided by a numerical calibration capability…

Cold start emissions challenge



Challenge

Catalyst heating mode



Catalyst heating mode

- Heat Transfer
- Species Evolution

ACEC Cold Start Protocol

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

Steady State Protocol

Transient Protocol

Experimental Approach – Coordinated Engine and Burner Experiments that Leverage Strengths of Each Laboratory

F.01.01 (Rockstroh) Pre-chamber cold start

E.01.01 (Curran) SCE CS & surrogate testing

E.01.02 (Sjöberg) Single-cylinder DISI CS Scoping

A.01.03 (Pitz) PAH Kinetics

Argonne F1. Accomplishments

- **Objective**
  - Investigation to highlight key engine and operating parameters for **advanced ignitor cold-start operability** **[task split across ACE 141]**
- **Approach**
  - Single-cylinder experiments with conventional and pre-chamber ignition systems
- **Technical Accomplishments**
  - Implemented enhanced engine test cell cooling system and conducted baseline SI cold start test according to ACEC test protocol.
  - Active pre-chamber system in process of commissioning.

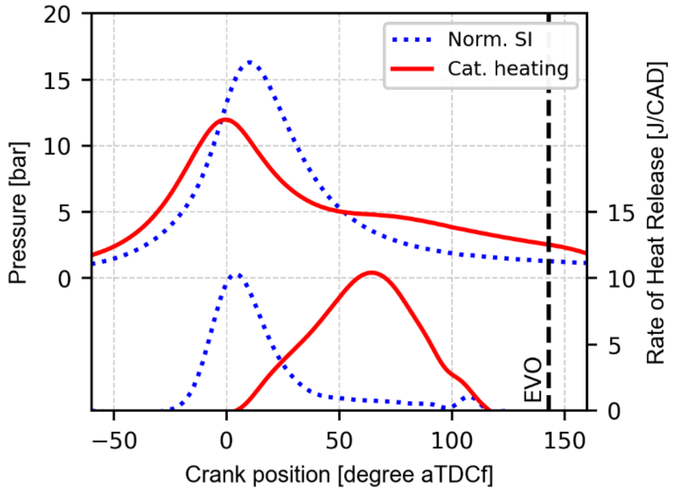
ANL Single-Cylinder Engine Geometry

CR (-)	12:1*
Disp. (L)	0.63
Bore x Stroke (mm x mm)	89.04 x 100.6
Injection	DI (central)

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

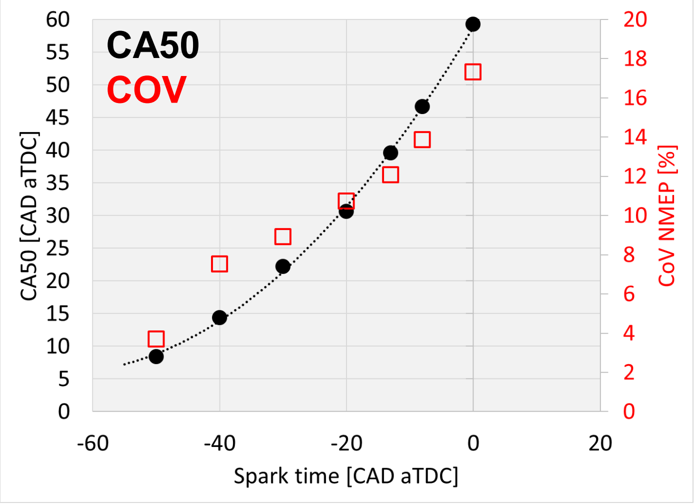


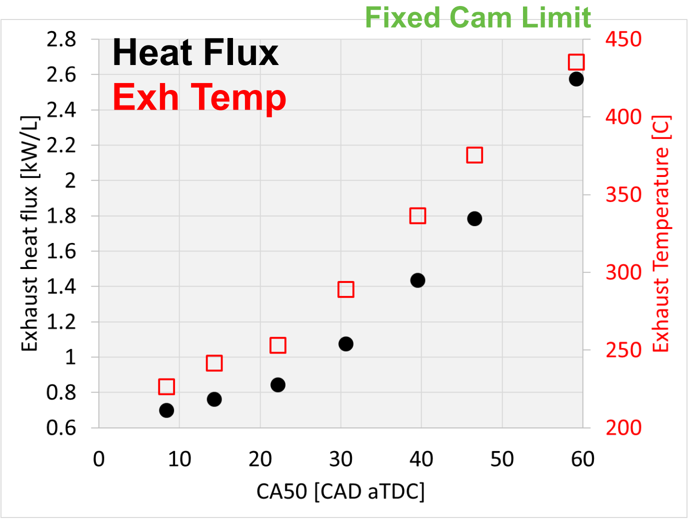
Argonne: Initial cold start protocol experiments completed

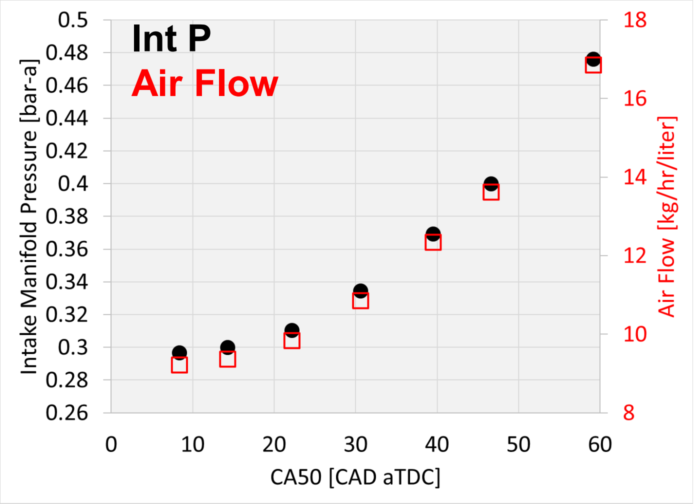
- **Cold start experiments** conducted using conventional spark ignition system according to ACEC protocol
  - ACEC defines heat flux sweep and boundary conditions
  - RD5-87 gasoline used
- Combustion phasing retarded to 60 aTDC
- Maximum exhaust heat flux of 2.6 kW/L and exhaust temperature ~430 C
  - Lower than prescribed heat flux – under discussion with ACEC – fixed Cam
  - **2.6 kW/L will be baseline for Pre-Chamber**

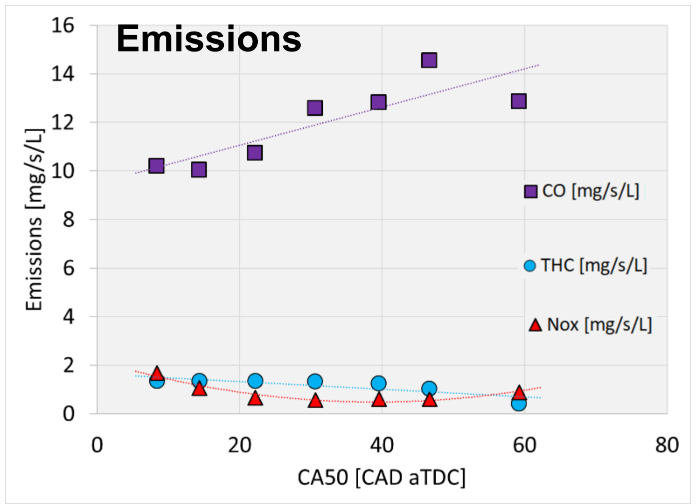
Provides a baseline for pre-chamber ignition system to be tested in passive and active configuration in next phase of experiments

Cold start experimental results – conventional spark ACEC protocol followed









Approach/Technical Accomplishments

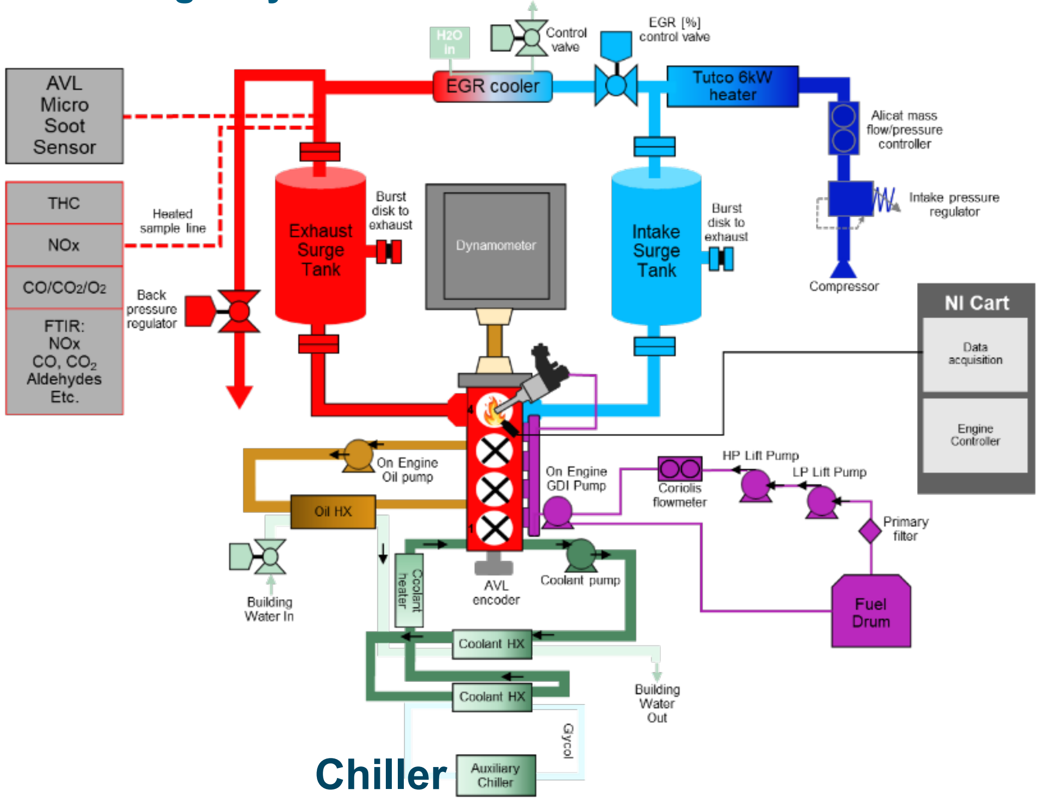
- **Objective:**
  - Develop comprehensive dataset about engine operation under cold start and warm re-start conditions for model validation, including exhaust heat flux, emissions, and thermal boundary conditions.
- **Approach:**
  - Single-cylinder engine experiments with GM LNF with detailed spatial exhaust measurements and detailed exhaust speciation – **ACEC Cold Start Protocol FY20**
- **Technical Accomplishments:**
  - Initial experiments completed with RD5-87 with simplified exhaust measurements and LLNL surrogate validation
  - Advanced exhaust measurement configuration underway for FY 20 experiments

PACE-1 [ACE139]

Quantity	RD5-87	LLNL Surrogate*
RON	92.3	92.3
MON	84.6	82.4
HC	2	1.98
Density	0.75	0.75
PMI	1.68	1.56**
T90	160	165

** Measured for ORNL blended surrogate – See Wagnon – ACE139*

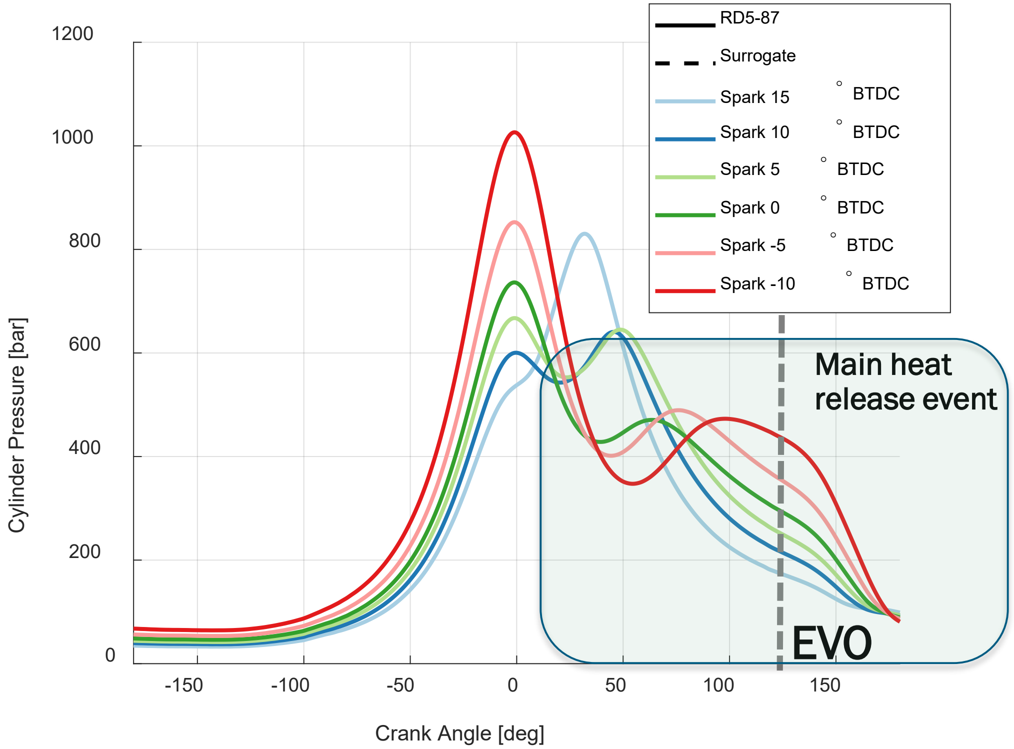
ORNL Single-Cylinder LD Platform for Cold-Start and Knock



Specification	(-)
Base engine	GM LNF
Bore x stroke:	86x86mm
Injection	DI – Side mount
Base CR	9.2:1
Firing cylinder	Cyl 4 (SCE config)

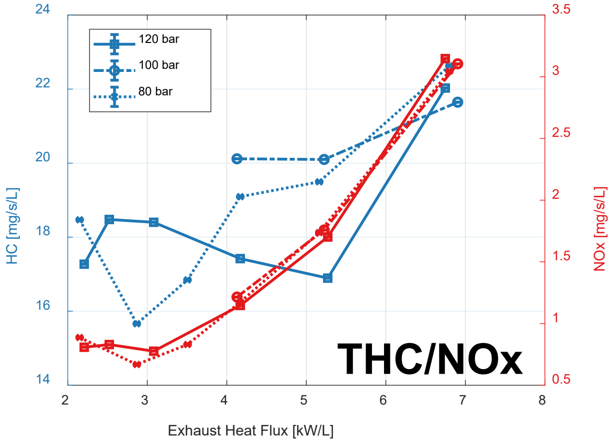
RD5-87 Cold-Start Baseline Experiments

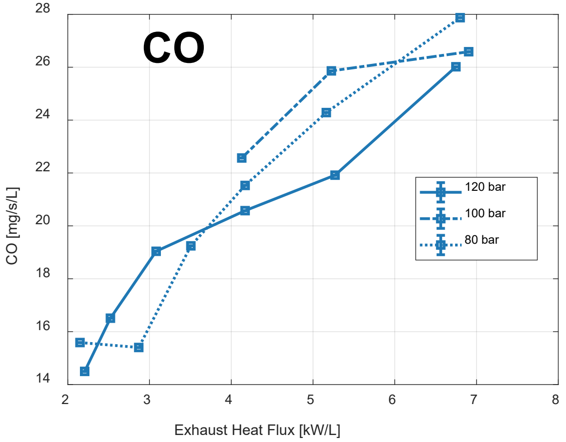
- **Spark timing and injection pressure effects evaluation**
- **Variable valve actuation available to extend heat flux range**
  - Exhaust heat flux range from 2-7 kW/L
- **HC, NOx, CO and Soot characterization**
  - Understanding of cold-start emission sources
  - Extensive validation data for model validation [ACE145]

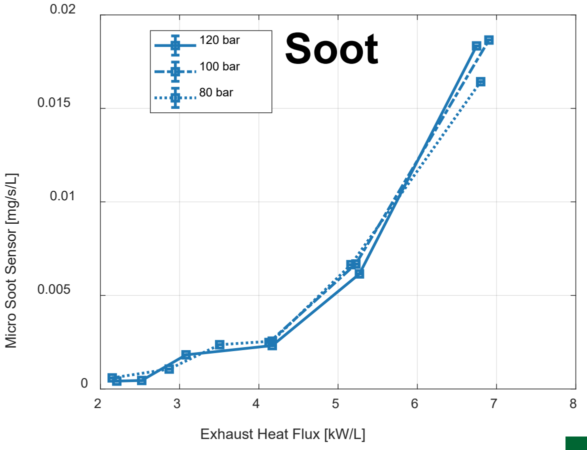


	RD5-87
Engine Conditions	ACEC Steady State Cold-Start Protocol
Injection Pressure [bar]	80,100 and 120
Spark Timing [°BTDC]	15, 10, 5, 0, -5 and -10
Injection Timing [°BTDC]	280
Lambda [-]	1
Cam Timings [°advance]	0 (int)/0(exh)

Characterization of Cold-Start performance with RD5-87 across multiple spark and injection pressure conditions





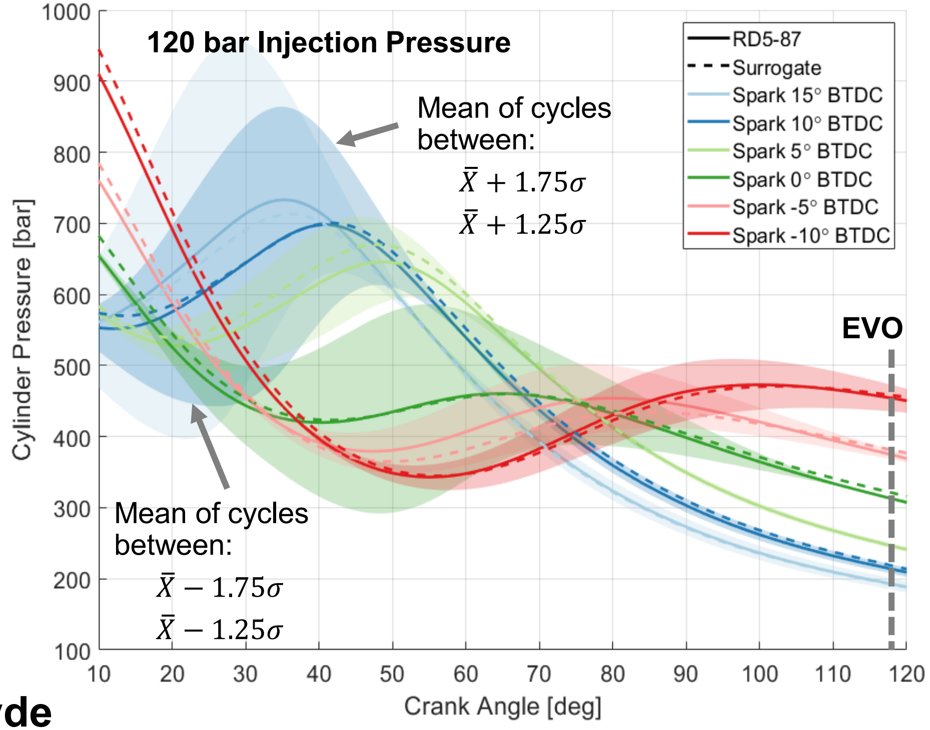


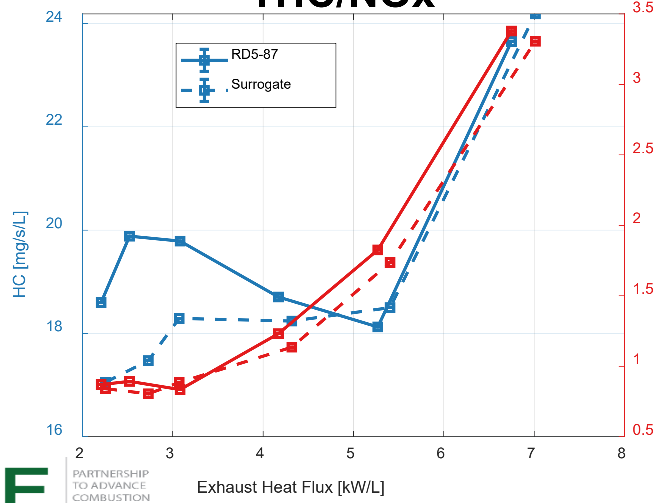
ORNL: PACE 1 Fuel Surrogate Experimental Validation

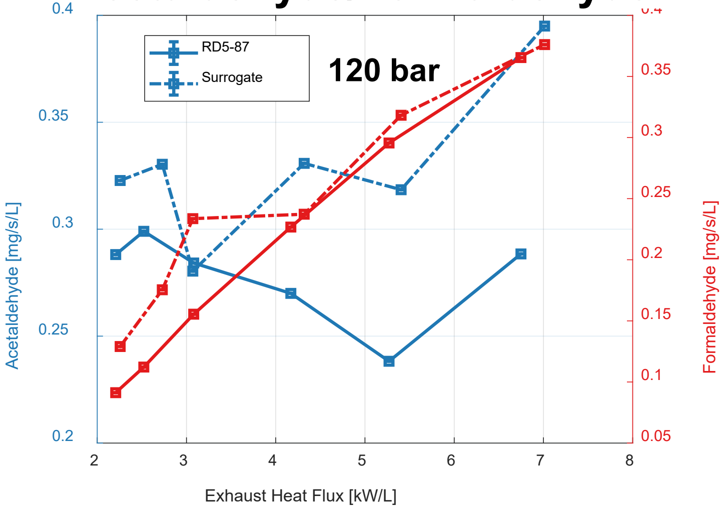
- **Single cylinder experiments compare LLNL PACE surrogate against RD5-87** [see Wagnon ACE 139]
  - Exhaust flux sweep following ACEC protocol (shown earlier)
  - Both fuels show the same combustion performance, within experimental variation, despite large cycle-to-cycle variation.
  - Emissions profiles across the exhaust heat flux range are well matched between fuels.

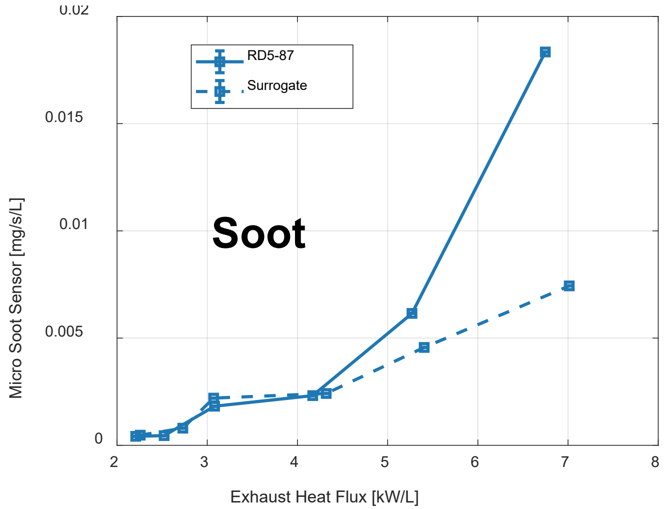
PACE surrogate successfully mimics the real full-boiling range fuel under cold-start conditions and can be used to predict engine performance and emissions

Supports PACE Outcome









SNL E.01.02 Accomplishments

Objective

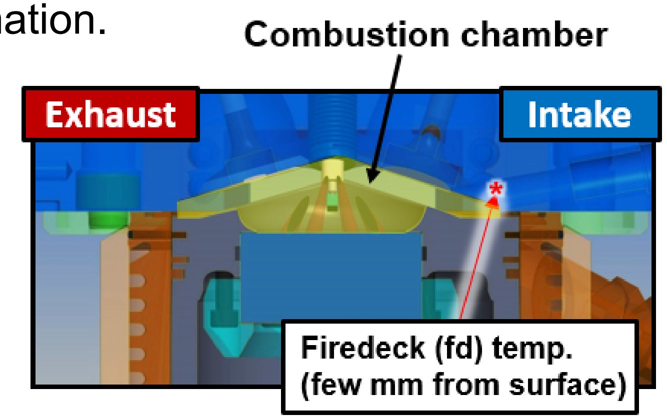
- CFD models need to capture key phenomena that lead to excessive PM throughout cold-starting and warm-up phases.
- Here, perform experiments to reveal relative importance of various pathways to soot formation.

Approach

- Operate engine at 1300 rpm. **Span thermal states from transient cold-start, to ACEC steady-state cold, to hot steady-state.**
  - Maintain exhaust ϕ= 1.
  - Measure coolant and firedeck temperatures.
- Assess effects of injection schedules and intake-flow configurations.
- Contrast E10 RD5-87 with various surrogates. Start with iso-octane, representing the simplest surrogate.
- Use PM/PN measurements to reveal relative importance of various factors that lead to soot formation.

  A. Imperfect bulk-gas mixture formation and free-flow soot formation.

  B. Fuel wall-films with diffusive combustion or pyrolysis.

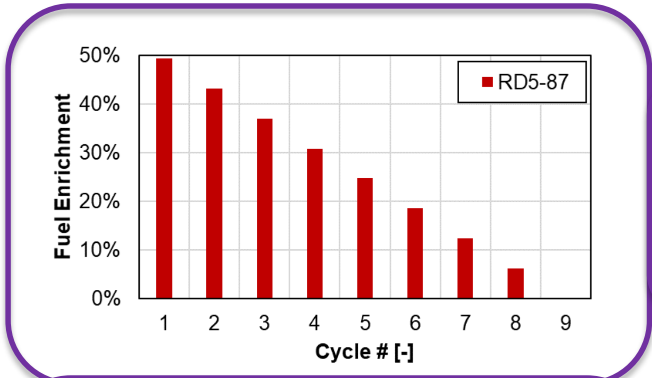


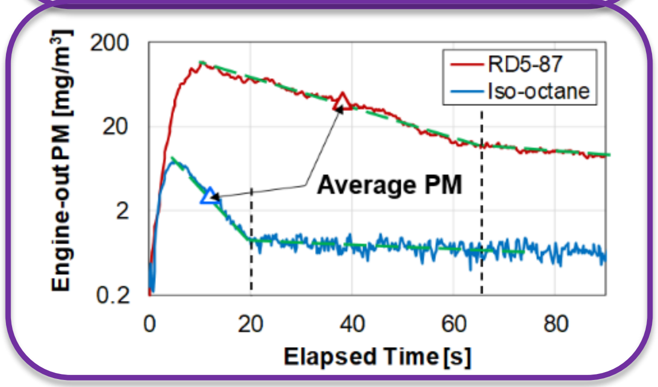
Technical Accomplishments

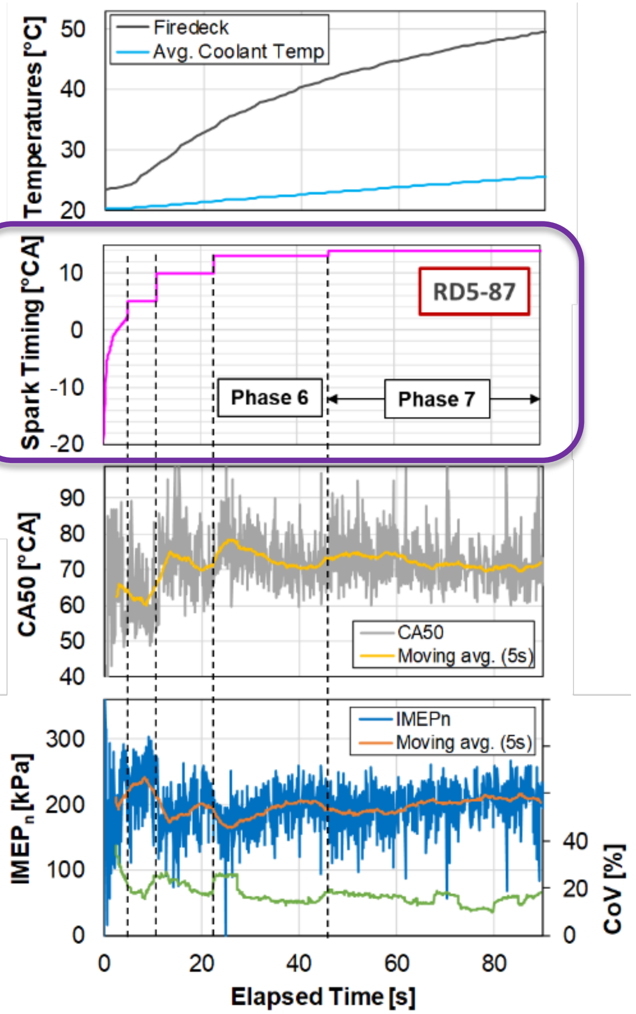
- Established numerous engine test protocols, measurements capabilities, and analysis procedures.
- Established catalyst-heating operation with exhaust enthalpy flow (>4.3 kW/L) and IMEP stability that meet ACEC guidelines.
- Determined that changes to in-cylinder surface fouling level can cause PM/PN to vary by factor of 10.
- Demonstrated that combined effects of fuel, fouling level, and thermal state cause PM to vary by factor of 4000.

Establishing and Comparing Test Protocols: Transient Cold-Start, Steady-State Cold, and 20/80 Skip-fired

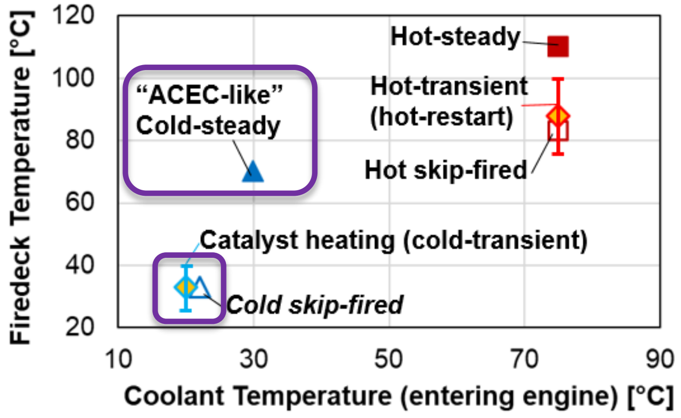
- **Transient cold-start operation** is most realistic. Uses enrichment for first 8 cycles and transient spark-timing.
- Most complex – requires analysis of transient PM/PN measurements.
- Low test throughput due to cold-soak time.



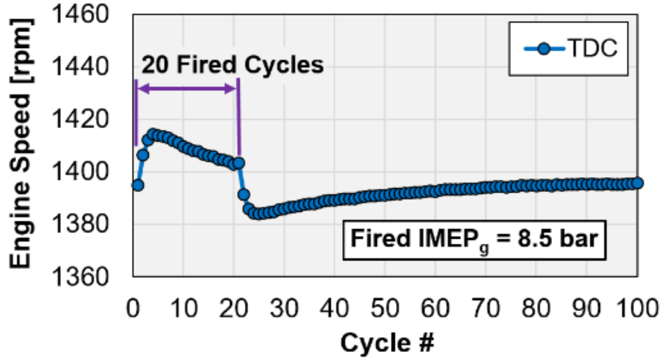




- **ACEC Cold Steady-State is easiest to implement**
- Continuous firing ⇒ high surface temperatures.
- Fails to fully capture PM cold-start challenge.

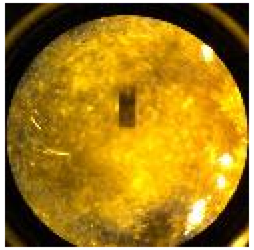


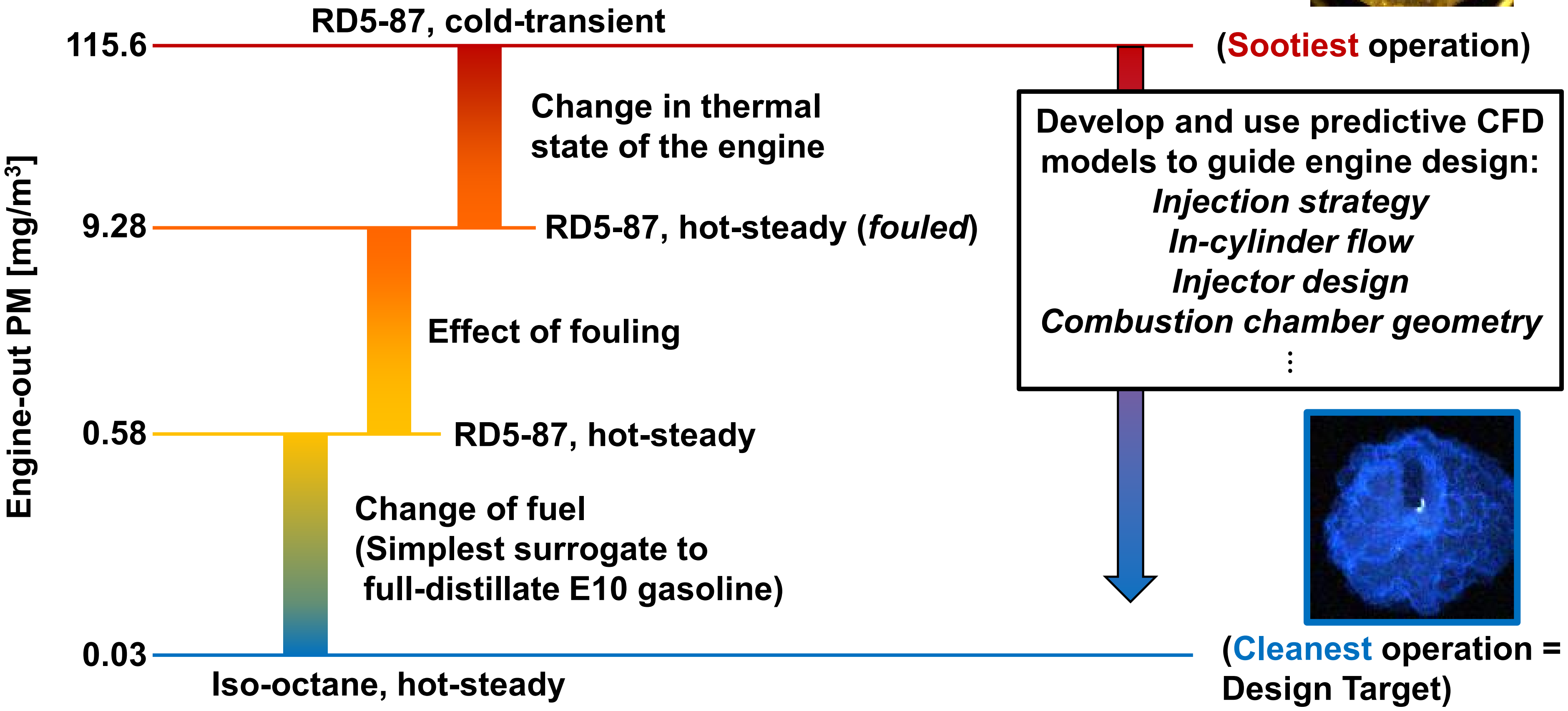
- **Skip-fired operation** can combine the best of both.
- 20/80 = 20% duty cycle ⇒ Low surface temperatures.
- "Unlimited" statistics for CFD validation.
- Requires a well-tuned dyno controller.



PM/PN Book-Ends Determined by Combinations of Thermal States, Fouling Levels and Fuels

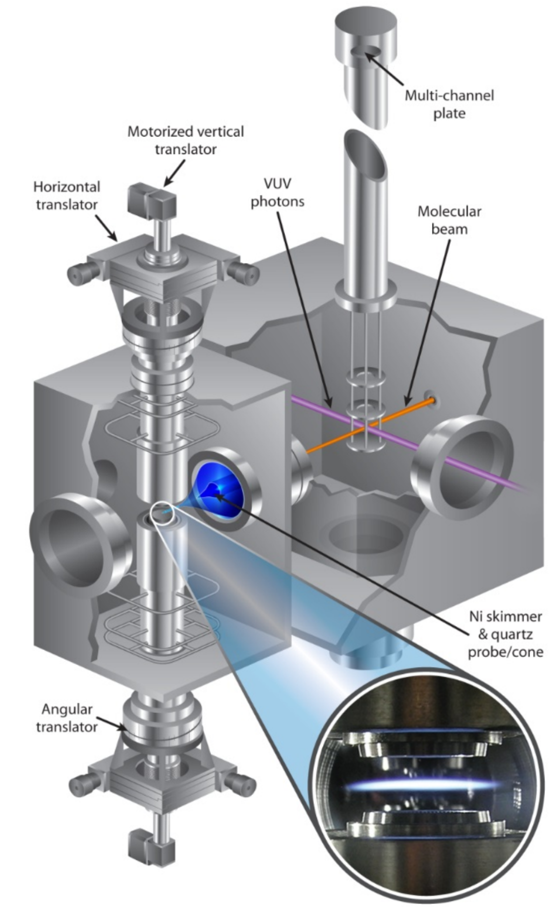
- The exhaust soot level varies by x 4000 when injection schedule is not adjusted to the optimal for each combination of thermal state and fuel type.
  - Here, use double injections with SOI_{a1} = -307°CA, SOI_{a2} = -293°CA.
- First CFD challenge may be to predict PM to the correct order of magnitude.





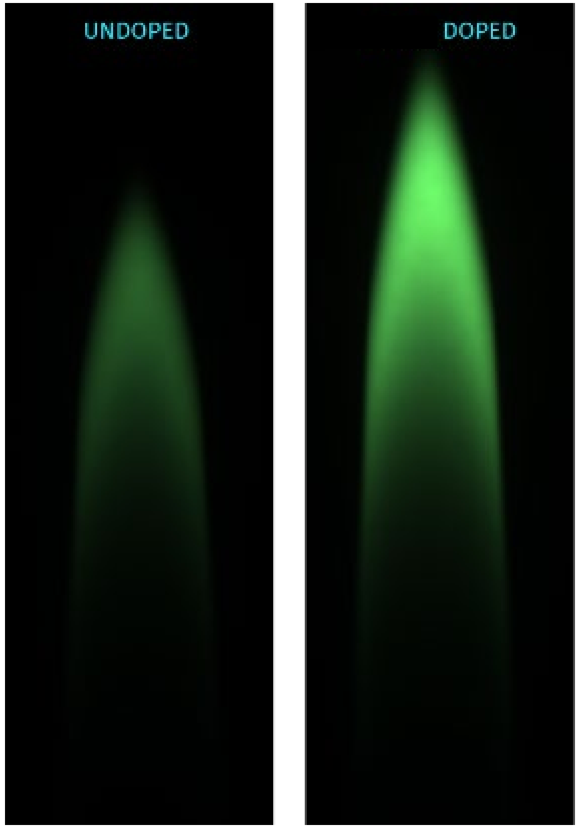
PAH mechanism validation against data from fundamental reactors

Sandia Counter-Flow burner

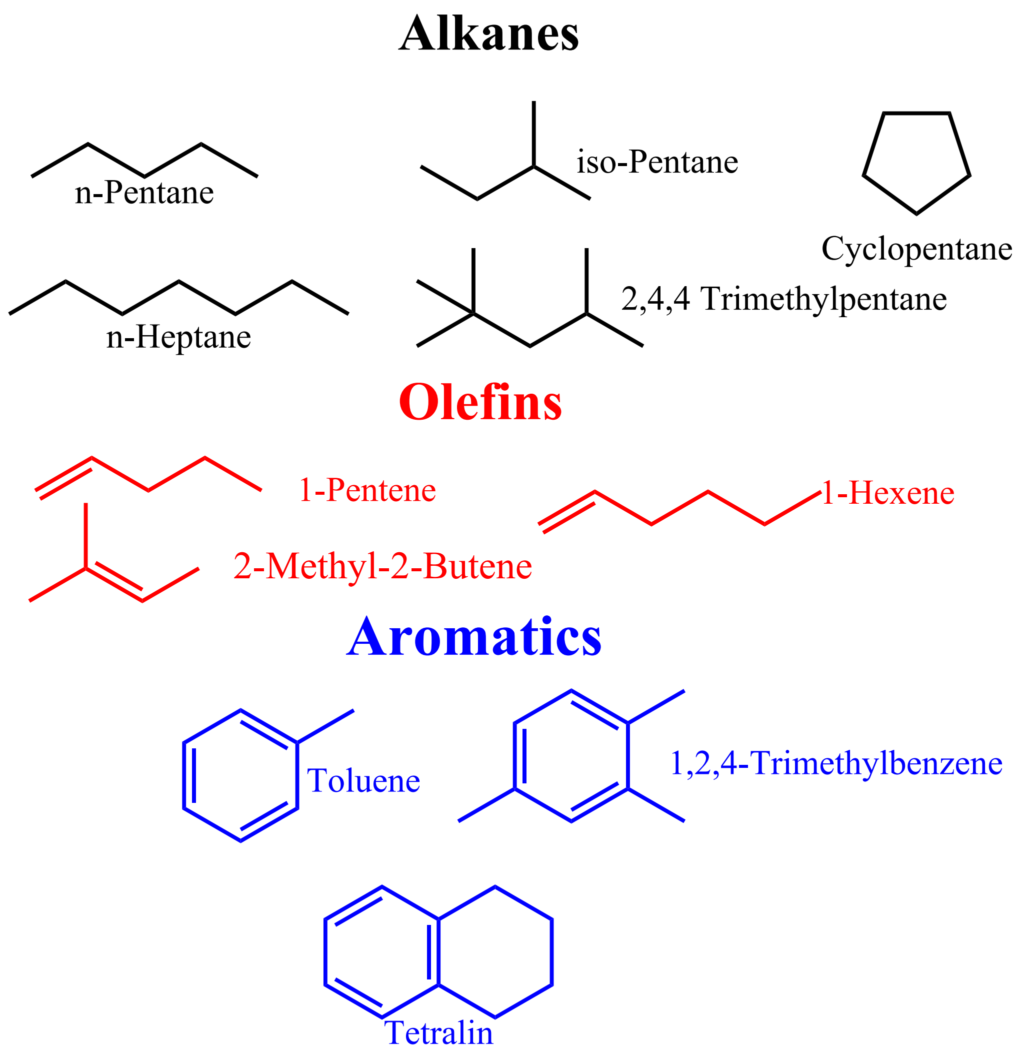


Validation mechanism against formation of PAH's in laminar counterflow diffusion flames of gasoline surrogate fuels

YSI measurements (Yale Univ.)

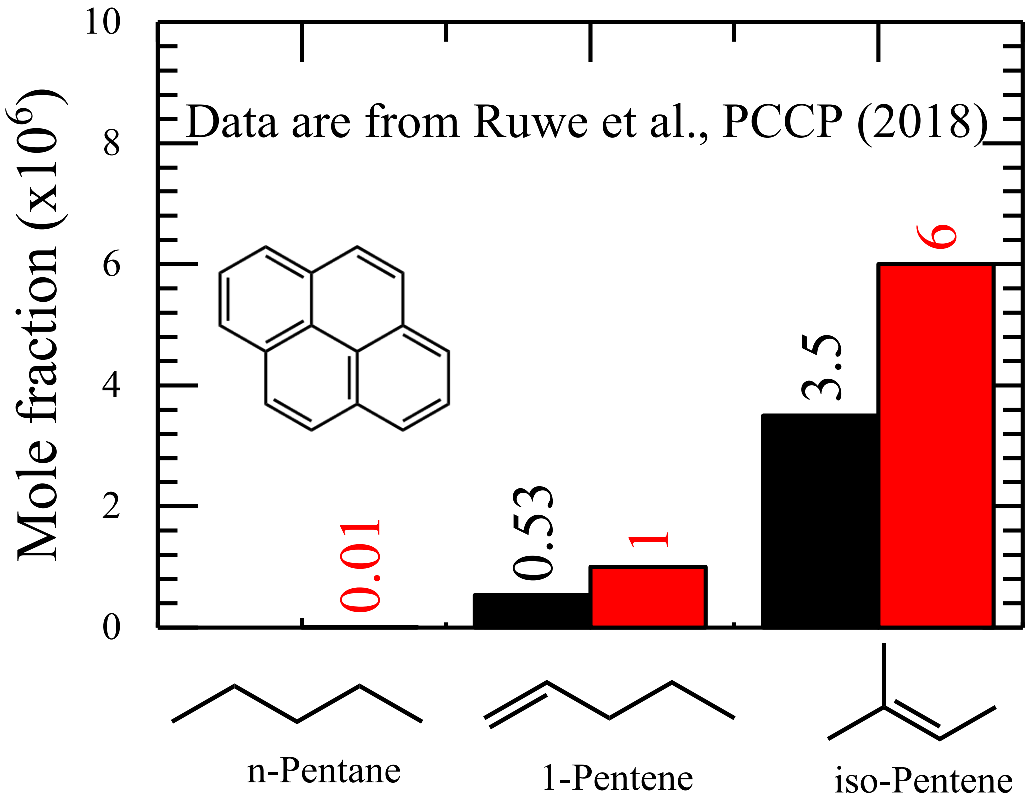


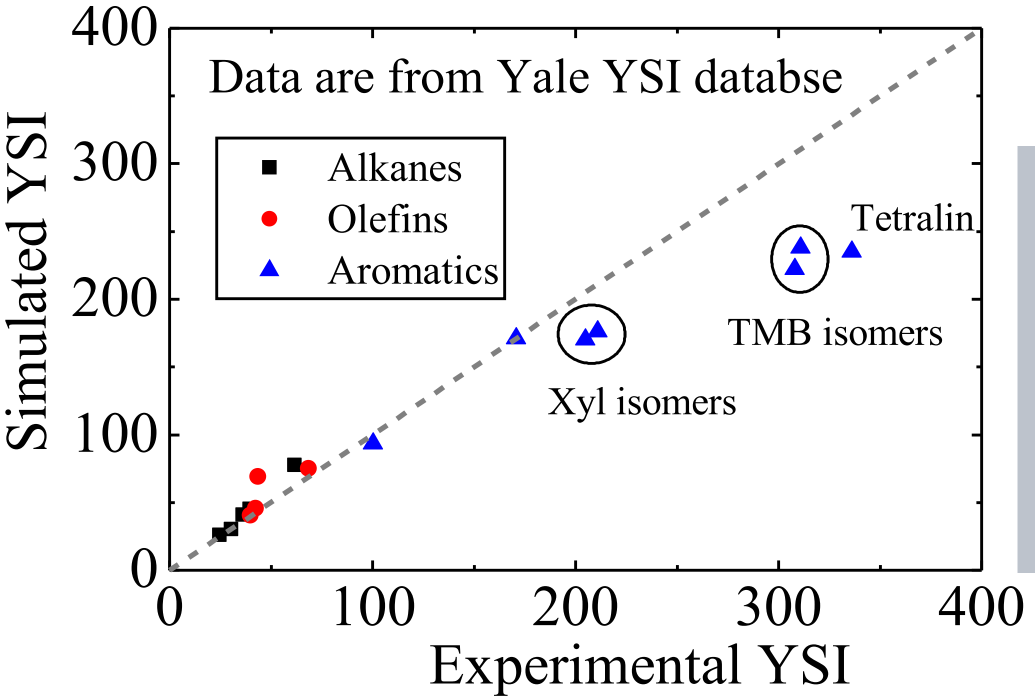
Comparison of Sooting tendency of gasoline surrogate fuels at a standardized condition.



YSI important for mechanism validation

Validation of PAH mechanism





YSI index computed and compared for all the molecules in the palette

Deviation for larger aromatics -> lack of understanding of pyrolysis chemistry of highly methylated aromatics

PAH mechanism validated against speciation data from flames and against a sooting metric for components in the gasoline surrogate palette

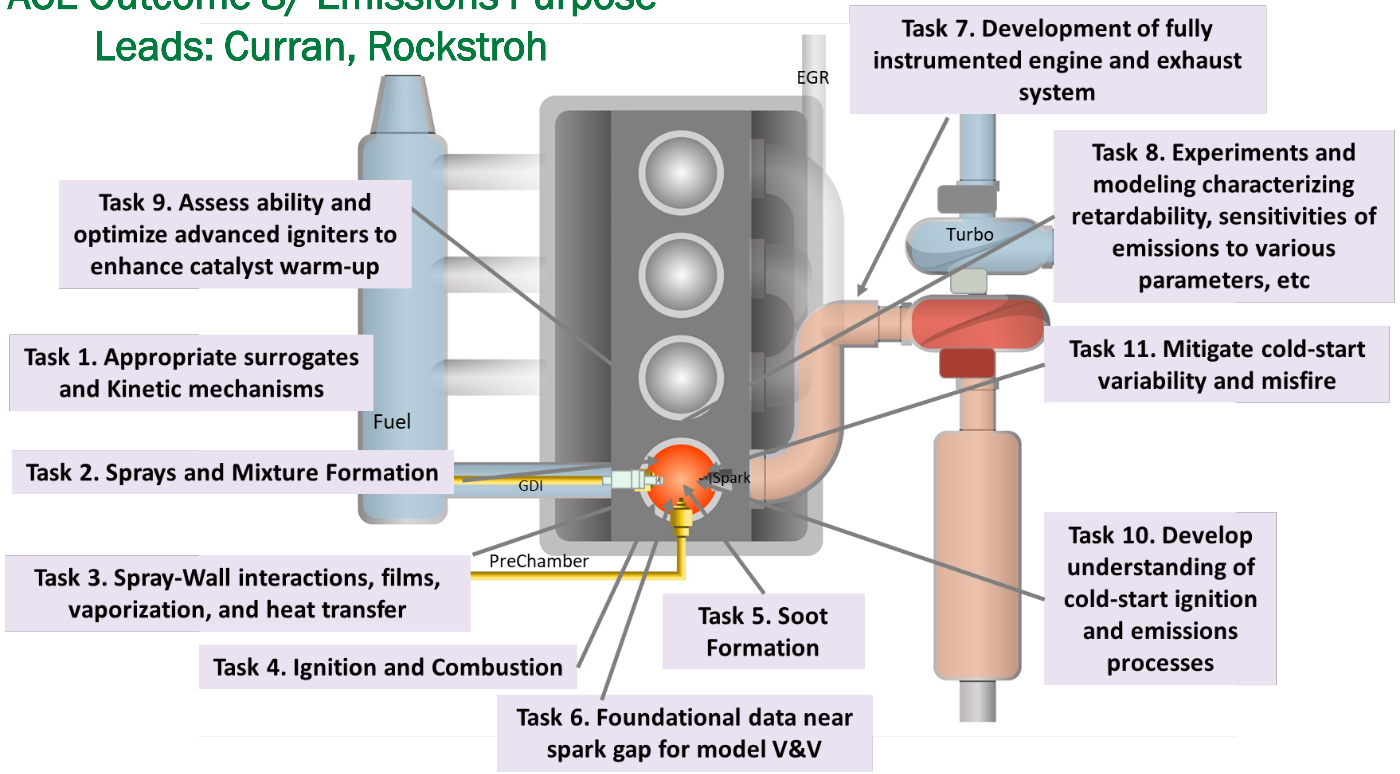
YSI simulations were conducted by S. Lapointe, LLNL

Responses to reviewer comments

- PACE projects were not reviewed in FY 19

COLLABORATION AND COORDINATION

PACE Outcome 8/ Emissions Purpose
Leads: Curran, Rockstroh



PACE

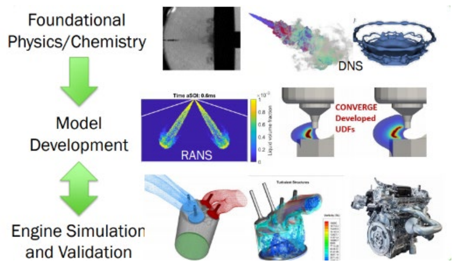
Purpose
Enable zero-impact tailpipe emissions aided by numerical capability

Major Outcome
Integrated assessment of cold-start modeling

Task Areas
11 tasks,
4 teams

Model Collaborations
Cold-start data sets for model validation

Improved Models



Component Models

Engine Models With CHT

Component data – matched engine conditions

Engine data – matched conditions

- PACE is a collaborative project of multiple National Laboratories…. **ACE 138**
- The work plan for PACE is developed in coordination with the USDRIVE ACEC Tech Team
- Partial list of individual collaborations for this project:
  - Co-Optima PI and Team Lead of Advanced Engine Development.
  - PACE activities not reviewed here: fuel surrogate selection & blending (Wagnon), and spray-film research (Pickett).
  - Collaborating with Xu He at Beijing Institute of Technology on fuel sprays, wall wetting and flame-speed measurements.
  - Collaborating with Charles McEnally at Yale on fuel sooting metrics.

Challenges and Barriers and Proposed Future Research

Purpose: Deeper understanding of cold-start physics to achieve faster, numerically-aided calibration

Task	Challenges/ Barriers
A.01.03 (Pitz) PAH Kinetics	Understanding of pyrolysis chemistry of trimethylbenzenes and complex gasoline surrogates.
E.01.02 (Sjöberg) DISI CS Scoping	CFD model validation is challenging due to multiple sources of exhaust soot.
F.01.01 (Rockstroh) Pre-chamber cold start	Develop mixture preparation and ignition strategies to enable cold-start operation with an active pre-chamber system (ANL)
E.01.01 (Curran) Cold start & surrogate testing	Understanding temporal and spatial enthalpy and emissions evolution post EVC
E.01.01 (Curran)	Limitations at steady state
PACE Outcome 8	Matched validation data

Proposed Future Research (selected)
Validation of PAH and soot model against data from Spray reactors..
Apply optical diagnostics to determine dominating soot-production pathways for selected operating conditions. Work with CFD modelers to validate sub-models one by one.
Parametric study to quantify pre-chamber volume and nozzle geometry effects on cold-start operation.
New exhaust manifold with sampling system for FY 20 experiments to complete additional data sets with high fidelity data [ACE148, ACE145]
FY 21 Pseudo transient protocol
Matched PACE Engines

~22 -FY20-23 Intermediate Milestones for Outcome 8

Outcome 8 | Purpose

Summary

Outcome 8 | Purpose

Relevance

- **US Drive Priority 1 Cold Start Barriers**
- PACE Outcome 8: **Purpose: Deeper understanding of cold-start physics to achieve faster, numerically-aided calibration**

Approach

- The work plan for Pace 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
- ACEC cold start protocol and PACE surrogate

Technical Accomplishments

- Delivering foundational science to improve understanding of cold-start physics and chemistry in combustion systems for emissions reduction
- Significant FY19/20 accomplishments going toward intermediate milestones

Collaboration and Coordination

- US DRIVE ACEC Tech Team, AEC MOU, Industry stakeholders
- 6 National Laboratories working towards common objectives
- Coordination and collaboration across PACE Consortium under Outcome 8

Proposed Future Research*

- FY 20 -23 plan with intermediate milestones to advance progress towards Outcome 8

Technical Backup Slides

Experimental Approach – Coordinated Engine and Burner Experiments that Leverage Strengths of Each Laboratory

PACE Major Outcome 8: Enable zero-impact tailpipe emissions aided by a numerical calibration capability…

F.01.01 (Rockstroh) Pre-chamber cold start

Metal single-cylinder engine

- Ford SCE GDI engine with prototype active pre-chamber
- Baseline spark advance sweep at 1300 / 2 bar - ACEC cold start protocol
- Conventional and pre-chamber ignition system

E.01.01 (Curran) SCE CS & surrogate testing

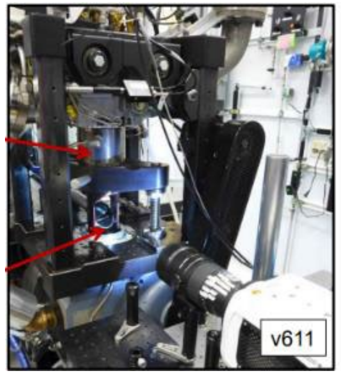
Metal single-cylinder engine

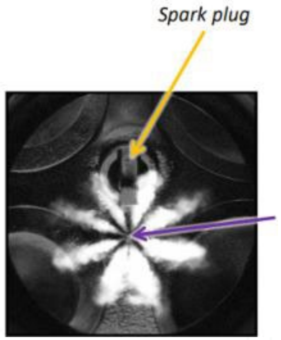
- GM LNF SCE – shared with Szybist knock task [ACE147]
- Chiller for ACEC cold-start protocol
- Comparison of RD5-87 with LLNL surrogate
- Speciation of exhaust + spatial enthalpy

E.01.02 (Sjöberg) Single-cylinder DISI CS Scoping

Metal & optical single-cylinder engine

- Stratified-charge capable, 0.55 L. Use early injections for well-mixed charge.
- First, conduct performance testing with all-metal engine over wide ranges of conditions.
- Second, apply optical diagnostics to determine dominating soot-production pathways.

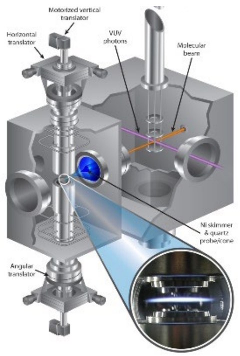


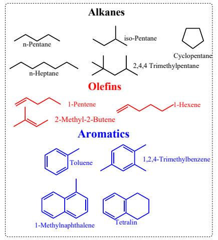


A.01.03 (Pitz) PAH Kinetics

Counter-Flow burner

- Validation mechanism against formation of PAH's in laminar counterflow diffusion flames of gasoline surrogate fuels
- PAH mechanism validation against data from fundamental reactors for deeper understanding of soot pathways





Using ACEC Cold Start Protocol and RD5-87 + PACE Surrogate

Linking Engine to Fundamental Soot

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**

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°BTDC to -10°BTDC to cover exhaust enthalpy space.
- Cams at maximum NVO (shown to result in better performance).
- Three injection pressures are evaluated to explore effects of mixture formation and wall wetting.

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	Surrogate
Engine Speed [rpm]	1300	
Coolant, Oil and Air Intake Temperature [°C]	20	
Load [NIMEP]	2	
Injection Pressure [bar]	80,100 and 120	80 and 120
Spark Timing [°BTDC]	15, 10, 5, 0, -5 and -10	
Injection Timing [°BTDC]	280	
Lambda [-]	1	
Cam Timings [°advance]	0 (int)/0(exh)	

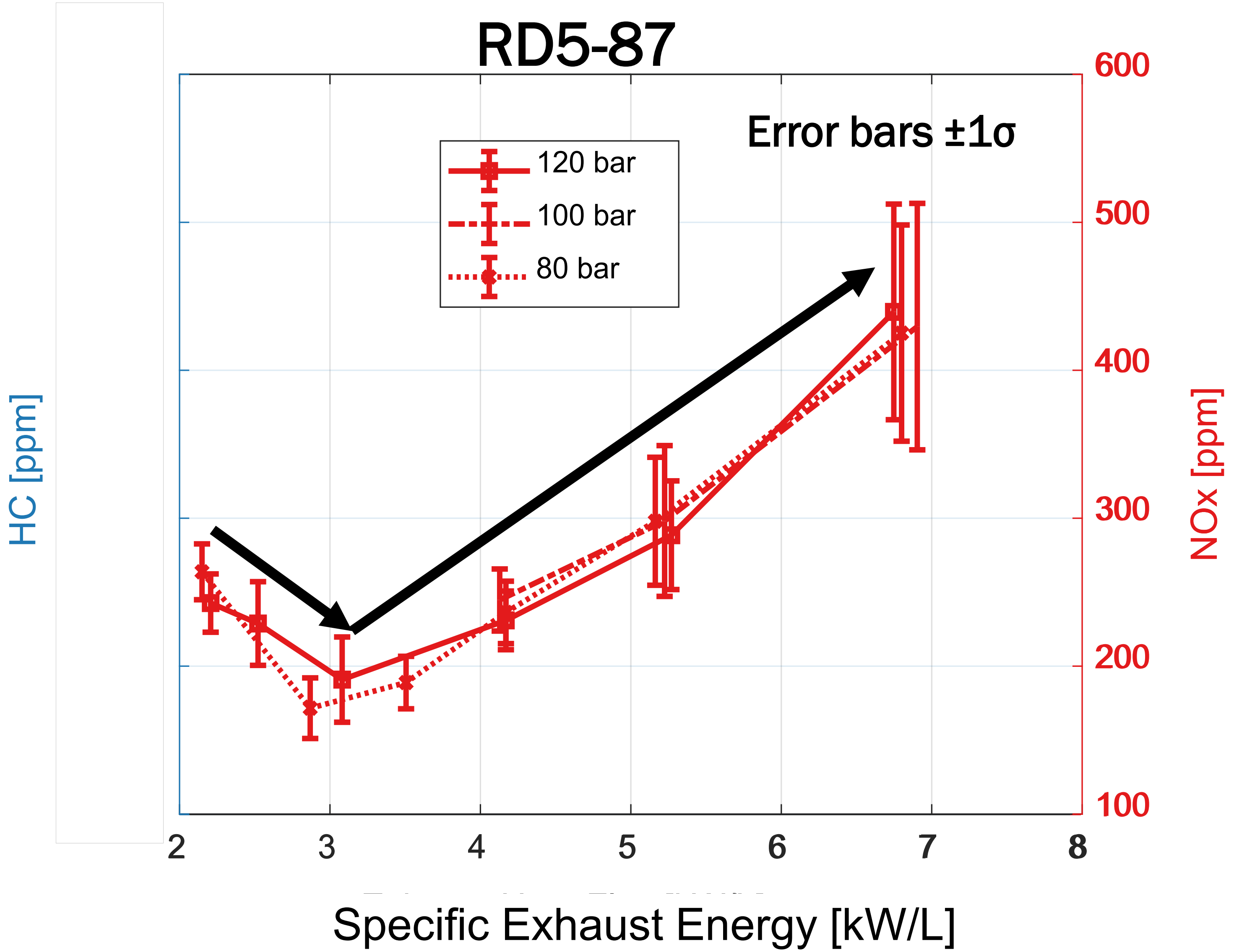
Technical Accomplishments: First PACE Cold-Start Datasets

Experiments were conducted by Flavio Chuahy, ORNL

- **First PACE Cold-Start datasets were collected in single-cylinder engine experiments (LNF):**
  - Initial spark retard reduces NOx
  - Further retard → Increase in late cycle peak temperatures due to lower thermal efficiency + reduction in trapped residuals due to hotter exhaust temperatures
  - Higher post-flame and exhaust temperatures enhance post-oxidation rate of unburned hydrocarbons
  - Second set of experiments planed for Q3/Q4 FY 20

PACE Surrogate and datasets available for cold-start baseline modeling effort →

Modeling approach evaluations
(Edwards ACE 145)



PACE-1 Surrogate successfully blended (ORNL blend)

- Samples sent for analysis

Component	Desired Mass %	Actual Mass %	Error %
n-heptane	17.13	17.12	-0.06
Iso-pentane	6.35	6.37	0.37
Iso-octane	19.89	19.90	0.05
1-hexene	5.97	5.97	-0.06
Cyclopentane	10.6	10.6	-0.03
1,2,4 - trimethylbenzene	30.11	30.09	-0.06
Ethanol	9.95	9.95	0.03

	RD5-87	Target Fuel Properties	PACE1-ORNL
IBP			44.4
T5			57.2
T10	57.8	68.8	59.4
T15			61.1
T20			62.2
T30			66.1
T40			78.3
T50	101.3	102.8	98.9
T60			106.7
T70			120.0
T80			154.4
T90	157.9	168.4	165.0
T95			165.6
FBP			165.6
DHA Results:			
iso-pentane		6.35	6.143
cyclopentane		10.6	10.152
1-hexene		5.97	5.782
n-heptane		17.13	17.032
iso-octane		19.89	20.04
1,2,4-trimethylbenzene		30.11	30.302
ethanol		9.95	10.215
sum		100	99.666

	RD5-87	Target Fuel Properties	PACE1-LLNL	PACE1-ORNL
RON	92.3	92.8	91.8	923
MON	84.6	84.4	82.3	82.4
RVP				6.32
LHV				41.812
Density at 15 C				0.7498
Carbon Wt %				82.52
Hydrogen Wt%				13.65
H/C				1.98497334
Ethanol wt%				9.74%
Total Aromatics wt%				32.00%
Total Olefins wt%				6.30%

PACE PARTNERSHIP TO ADVANCE COMBUSTION ENGINES