

# Fundamental Advancements in Pre-Chamber Spark Ignition and Emissions Control for Natural Gas Engines

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DOE Vehicle Technologies Program  
2019 Annual Merit Review and Peer Evaluation Meeting

Project ID # FT080

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# Overview

## Timeline

- Project start date: 10/1/2017
- Project end date: 12/31/2019
- Percent complete: ~66%

## Budget

- Total project funding: \$3M
  - DOE share: \$3M
  - Contractor share: \$0
- Funding from FY 2018
  - Equally split amongst ANL/NREL/ORNL/SNL at \$750K each for total project

ANL: Argonne National Laboratory  
NREL: National Renewable Energy Laboratory  
ORNL: Oak Ridge National Laboratory  
SNL: Sandia National Laboratories

## Barriers / Technical Targets

- Natural gas engines need to improve dilution tolerance and lean operation to achieve diesel-like efficiency
- Fundamental understanding (physics, thermodynamics, and chemistry) is necessary for improving natural gas combustion efficiency
- Fundamental catalysis research for methane conversion is needed due to challenge of methane activation

## Partners

- ANL / NREL / ORNL / SNL
- Industry collaboration:
  - Altronic
  - Analytik-Service Gesellschaft (ASG) mbH
  - MAHLE
  - Daimler Trucks North America (Detroit Diesel)

# Relevance

- DOE Vehicle Technologies Office (VTO) has specific input regarding natural gas (NG) engine research needs for efficiency and emissions
  - Annual Natural Gas Vehicle Technology Forum
  - Natural Gas Vehicle Research Workshop (July 2017), which fed VTO's funding opportunity announcement (FOA) and the Lab Call that resulted in this multi-lab project
- Key high-level NG engine research needs:
  - Research needed to address **barriers for achieving diesel like efficiency** for NG engines
  - Ignition technology to enable ultra-lean operation (**pre-chamber**, volumetric ignition)
  - Fundamentals for improving NG combustion efficiency (**physics, thermodynamics and chemistry**)
  - **Low temperature combustion** (LTC) concepts conceivable for NG engines, ensure real-world mode switching and emissions control compatibility
  - Advances in computational fluid dynamics (**CFD**) and modeling for NG engines
  - Avoiding knock and **abnormal combustion** (i.e. low speed pre-ignition)
  - Fundamental catalysis research for methane conversion is needed due to **challenge of methane activation**
  - Research needed for both stoichiometric and **lean engine (LTC and conventional) emission control**

# Relevance

**This project focuses on early stage research focusing on pre-chamber spark-ignition (PCSI)** to achieve diesel-like efficiency in medium duty (MD) and heavy duty (HD) NG gas engines by extending the lean dilution limit and/or exhaust gas recirculation (EGR) dilution limit, as well as shortening burn duration, with integrated aftertreatment

## **Impact:**

This project integrates experimental and simulation based tasks to address four key barriers to market penetration of PCSI for MD/HD NG engines:

**Barrier 1** – **Inadequate science base and simulation tools to describe/predict the fluid-mechanical and chemical-kinetic processes governing PCSI** to enable engineers in industry to optimize designs for efficiency, noise, reliability, pollutant formation, emissions control integration, and drivability

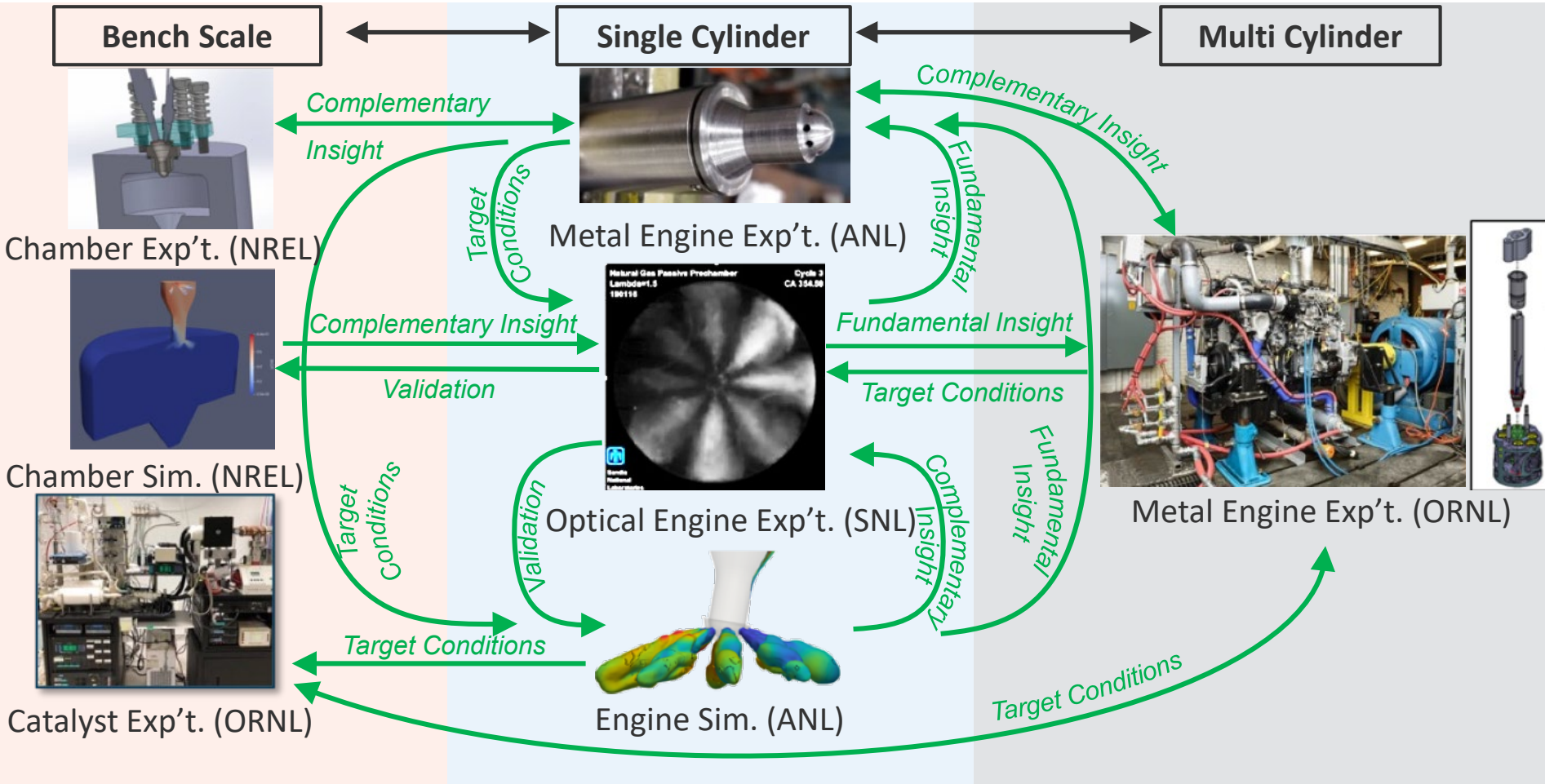
**Barrier 2** – Limited ability to **extend EGR and/or lean dilution limits** at higher loads

**Barrier 3** – Increased propensity for PCSI **hot-spot pre-ignition** at high loads relative to spark ignition

**Barrier 4** – **Ineffective methane catalysts** for the high engine-out unburned fuel concentrations coupled with low exhaust temperatures ( $<400\text{ }^{\circ}\text{C}$ ) of high efficiency engines

# Approach

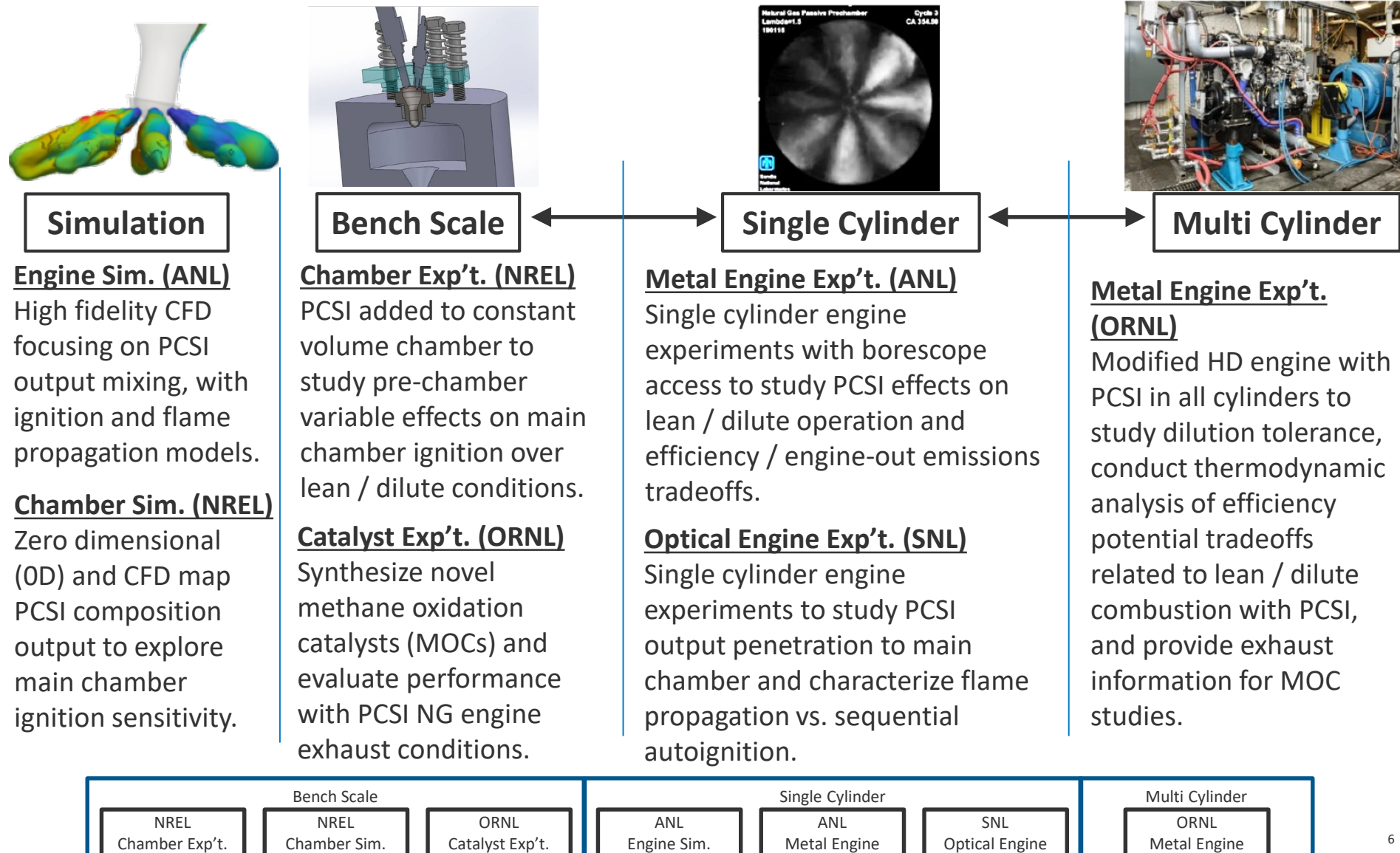
*Collaboration and integration across four national labs connect fundamental experiments and modeling to practical hardware*



*DOE laboratory expertise and capabilities focus on early-stage research to address key barriers for NATURAL GAS engines*

# Approach

Modular PCSI designs with as much commonality as possible are used across all platforms



# Approach - Milestones

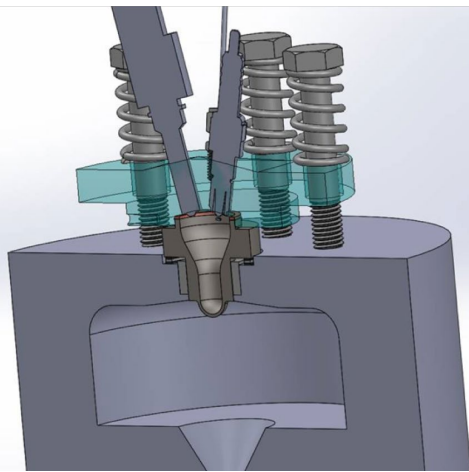
***A subset of key milestones are presented. The ANL / NREL / ORNL / SNL team meet semi-monthly to coordinate research tasks and share results. VTO updates are also coordinated.***

Date	Description of Milestone	Status	Lab
March 2018	Select synthesis strategy for improved MOC performance	Complete	ORNL
Sept. 2018	Single cylinder research engine configuration completed	Complete	ANL
Sept. 2018	PCSI combustion model evaluation to define what models are suitable for PCSI simulation	Complete	ANL
Dec. 2018	Initial in-cylinder ignition combustion optical imaging	Complete	SNL
March 2019	PCSI scoping experiments in Advanced Fuel Ignition Delay Analyzer (AFIDA)	Complete	NREL
March 2019	Single-cylinder data collection and post-processing	Complete	ANL
June 2019	Initial sensitivity analysis completed using OD or CFD simulations based on PCSI AFIDA experiments	On-track	NREL
Sept. 2019	Complete multi-cylinder engine dilution tolerance studies	On-track	ORNL
Sept. 2019	Presentation describing progress toward a conceptual model description of in-cylinder PCSI processes	On-track	SNL
Dec. 2019	Combustion model validation against experimental engine and optical data	On-track	ANL

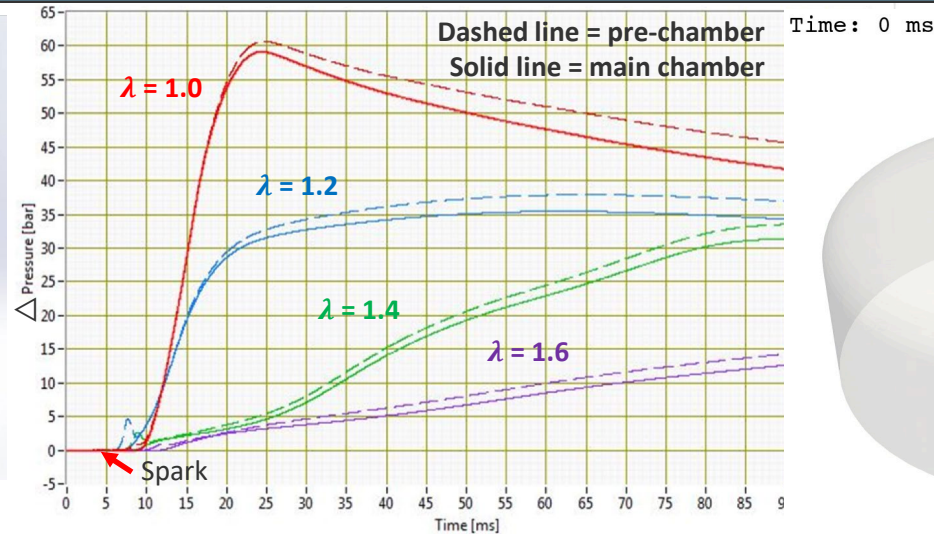


# Technical Accomplishments and Progress

Constant volume PCSI experiments and OD + CFD simulations provide sensitivity studies

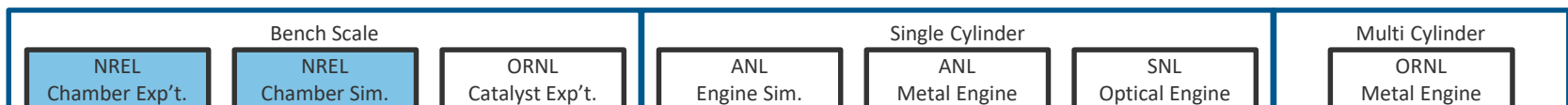


$\lambda$  = Lambda, air-fuel equivalence ratio  
ms = Milliseconds



OH: Hydroxyl radical    CH<sub>2</sub>O: Formaldehyde    O: Oxygen (elemental)    H: Hydrogen (elemental)

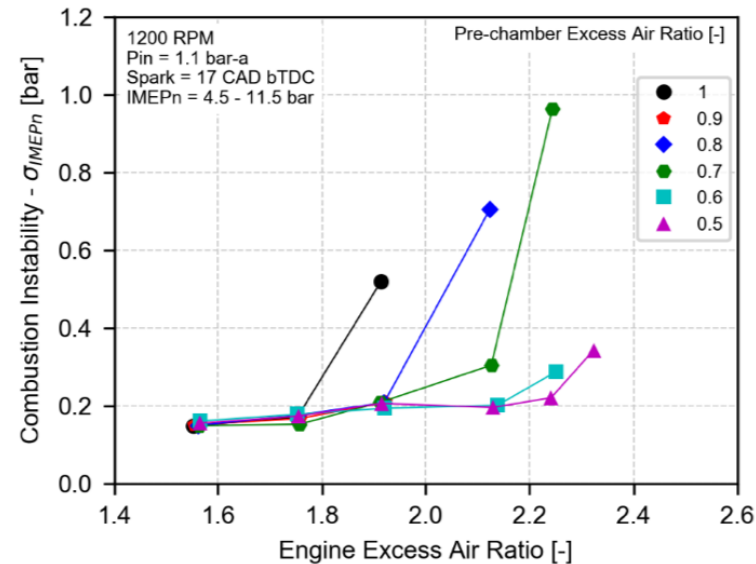
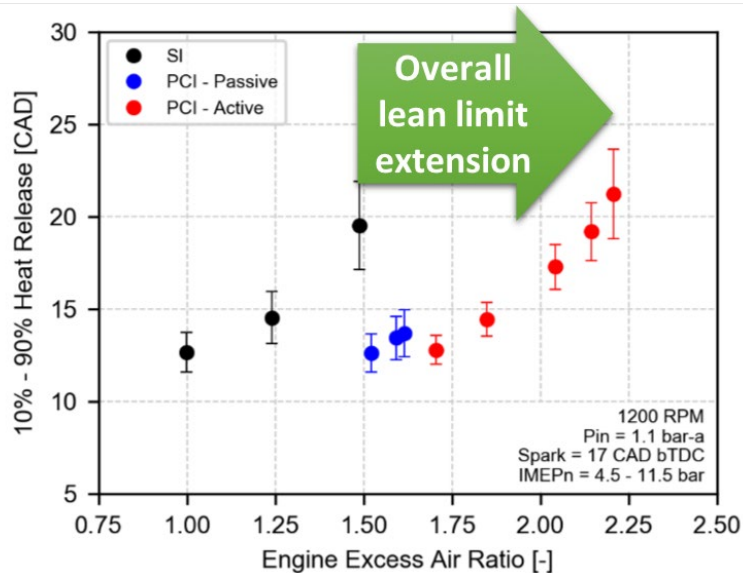
- NREL modified the AFIDA for studies of PCSI and main chamber pressure rise and ignition progress with well controlled temperatures and pressures, sweeping equivalence ratio and simulated EGR rates, providing guidance for SNL optical and ANL + ORNL metal engine experiments
- OD and CFD simulations map variations in PCSI jet composition to variations in flame speeds and ignition propensity, producing sensitivity factors for main chamber ignition quality in terms of mixture composition
- Initial results indicate OH, CH<sub>2</sub>O, O, & H radical pool output in jets are most critical to ignition





# Technical Accomplishments and Progress

Engine experiments show rich pre-chamber extends lean limits, with chemically active jets



bTDC: Before top dead center

CAD: Crank angle degrees

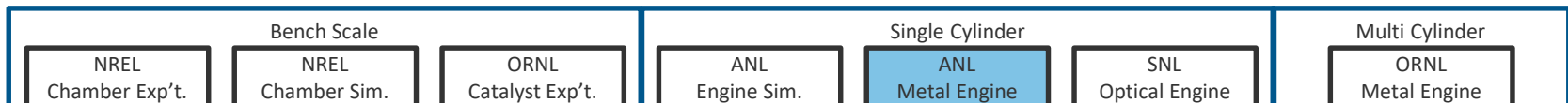
IMEPn: Net indicated mean effective pressure

PCI: Pre-chamber ignition

RPM: Revolutions per minute

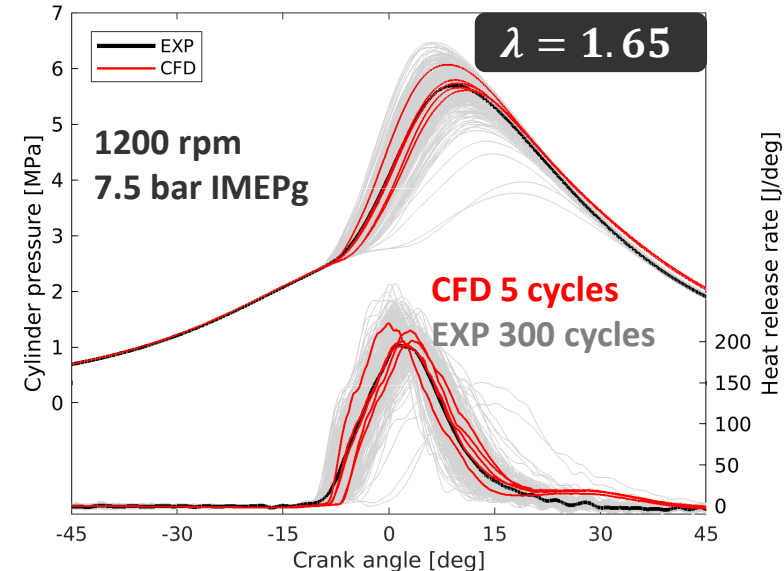
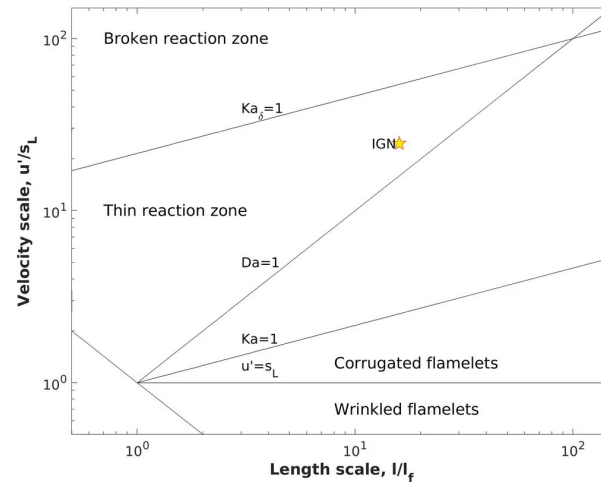
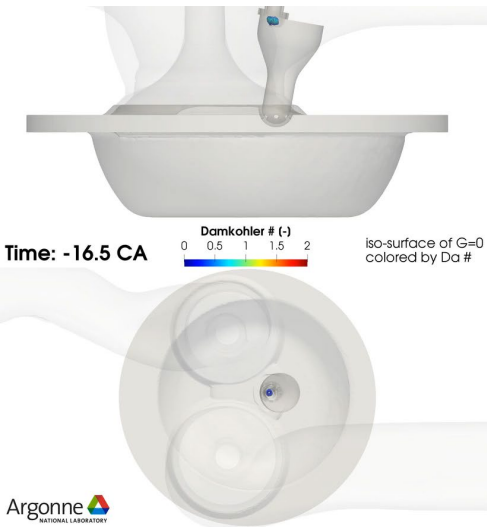
SI: Spark ignition

- ANL metal single cylinder engine studies demonstrated passive PCSI fueling extended lean limit to  $\lambda = 1.6$  (with same combustion duration / stability of SI)
- Active PCSI fueling significantly extended the lean flammability limit and enabled stable combustion at  $\lambda > 2.2$  by leveraging fuel-rich mixture inside the pre-chamber
- Lean limit extension beyond  $\lambda \sim 1.8$  required fuel-rich mixture inside the pre-chamber, but strength of rich mixture had no observed influence within the flammability limits
- Results suggest fuel-rich pre-chamber produces chemically active jets that ignite lean charge



# Technical Accomplishments and Progress

Engine simulations developed to accurately predict PCSI NG engine combustion

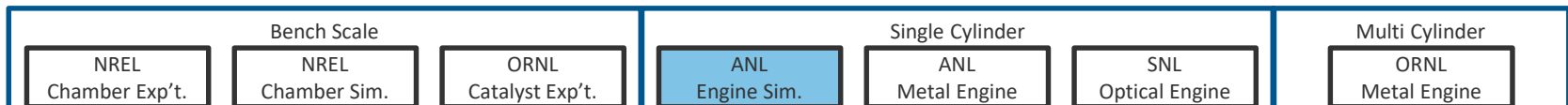


CA: Crank angle deg: Degrees

J: Joule

Da: Damkohler number IMEPg: Gross indicated mean effective pressure Ka: Karlovitz number MFB: Mass fraction burned MPa: Megapascals s: Seconds

- ANL simulations in CONVERGE showed G-Equation has higher potential to capture pre-chamber combustion events compared to other models (multi-zone well-stirred reactor; extended coherent flame model)
- G-Equation can account for both large and scale turbulences found in the pre-chamber, and these factors were tuned to match experiments at two operating conditions
- Strong turbulence-chemistry interaction is expected when jets exit pre-chamber ( $\sim 1\%$  MFB), and flame propagation dominates at very late stages



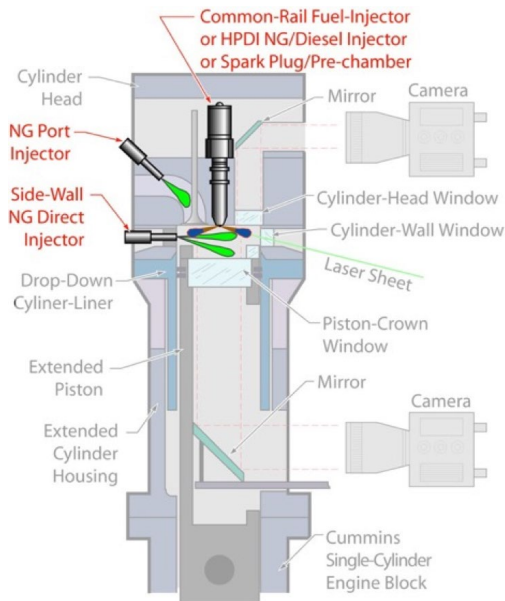
# Technical Accomplishments and Progress

B1: Science base




B2: Dilution

B3: Pre-ignition

Optical engine studies provide fundamental NG mixing and combustion data with PCSI

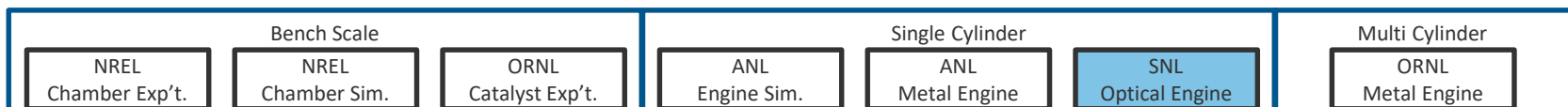


Visible combustion luminosity (broadband chemiluminescence, no filtering)

Lambda = 1.5		Lambda = 1.7		Lambda = 1.9	
Natural Gas Passive Prechamber Lambda=1.5 190116	Cycle 3 CA 350.00	Natural Gas Passive Prechamber Lambda=1.7 190116	Cycle 3 CA 350.00	Natural Gas Passive Prechamber Lambda=1.9 190116	Cycle 7 CA 350.00
					
Sandia National Laboratories		Sandia National Laboratories		Sandia National Laboratories	

COV: Coefficient of variation    IMEP: Indicated mean effective pressure    SCE: Single cylinder engine

- Initial studies with passively fueled pre-chamber reveal large cycle-to-cycle variation in timing of individual pre-chamber jet ignition even when COV of IMEP is low
- At leaner conditions, pre-chamber jet luminosity becomes increasingly variable, and main chamber combustion progression slows and becomes less flame-like and more distributed
- SNL experiments validate/inform NREL constant volume chamber and ANL SCE studies / simulations, and support development of a conceptual-model description of PCSI



# Technical Accomplishments and Progress

B1: Science base

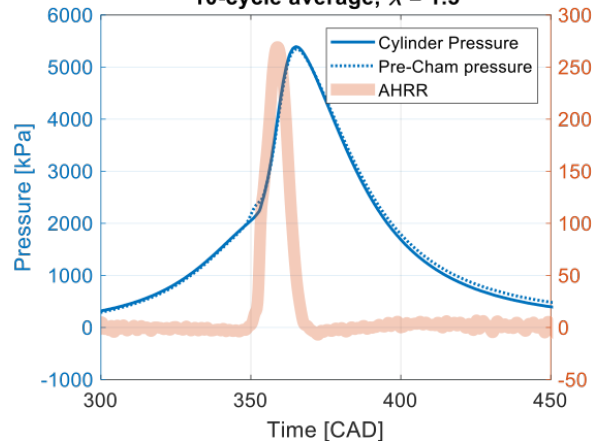
B2: Dilution

B3: Pre-ignition

Optical engine studies provide fundamental NG mixing and combustion data with PCSI

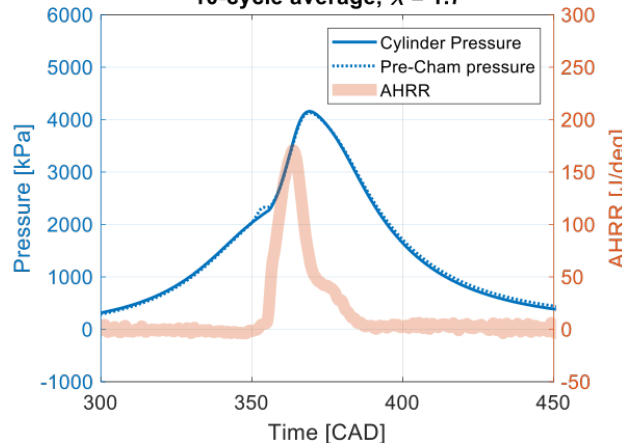
Lambda = 1.5

10-cycle average,  $\lambda = 1.5$



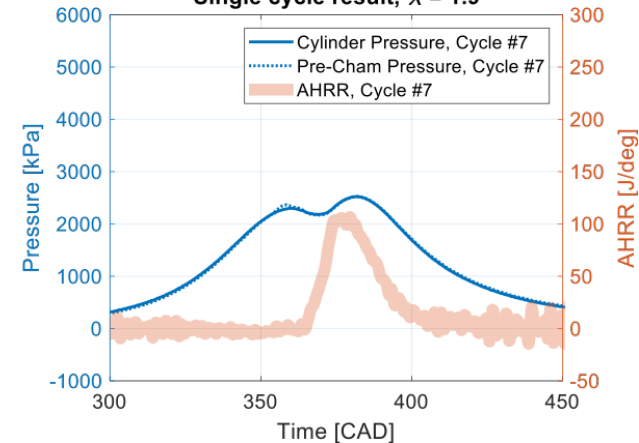
Lambda = 1.7

10-cycle average,  $\lambda = 1.7$



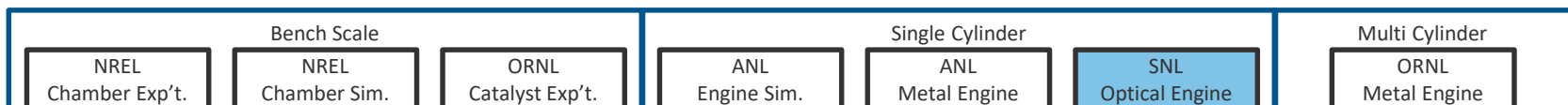
Lambda = 1.9

Single cycle result,  $\lambda = 1.9$



AHRR: Apparent heat release rate    kPa: Kilopascals

- Initial studies with passively fueled pre-chamber reveal large cycle-to-cycle variation in timing of individual pre-chamber jet ignition even when COV of IMEP is low
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# Technical Accomplishments and Progress

B1: Science base

B2: Dilution

B3: Pre-ignition

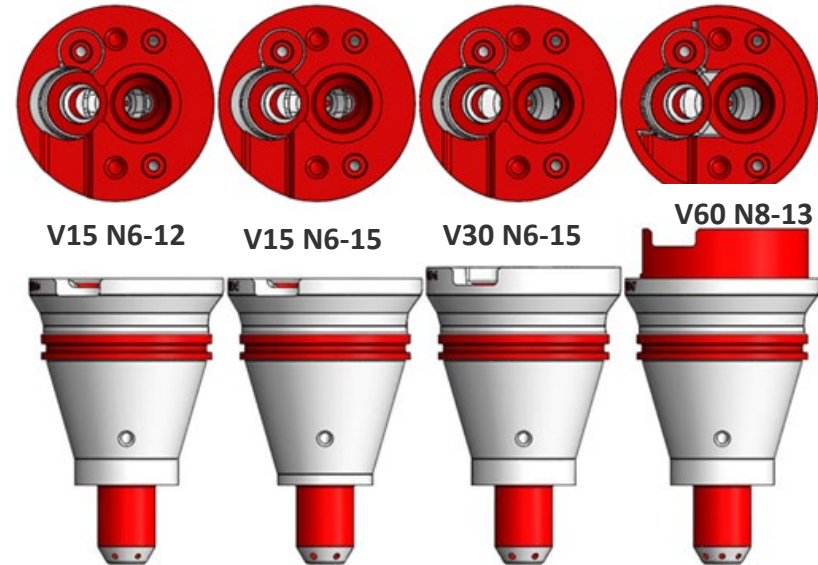
PCSI adapted multi-cylinder engine enables dilution tolerance and thermodynamic studies

## Prototype MAHLE PCSI modules

	V15 N6-12	V15 N6-15	V30 N6-15	V60 N8-13
Volume	1.5 cc	1.5 cc	3.0 cc	6.0 cc
# of nozzle holes	6	6	6	8
Nozzle hole diam.	1.2 mm	1.5 mm	1.5 mm	1.3 mm

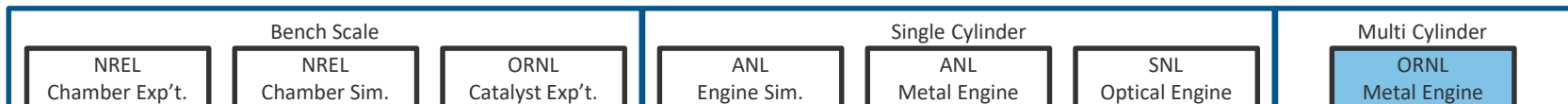
- ORNL adapted a prototype modular MAHLE PCSI design to the DD13... a robust system with engineering support was necessary, while still allowing links to ANL metal and SNL optical single cylinder engine studies, and ANL simulations
- **Focused dilution tolerance studies** will link with single-cylinder studies and simulations
- **1<sup>st</sup> and 2<sup>nd</sup> law studies** will provide insight on how PCSI shifts thermodynamic balances and to understand what additional opportunities for improved efficiency exist
- Will provide **exhaust composition data to MOC study**

## Pre Chamber Bodies for MCE DD13



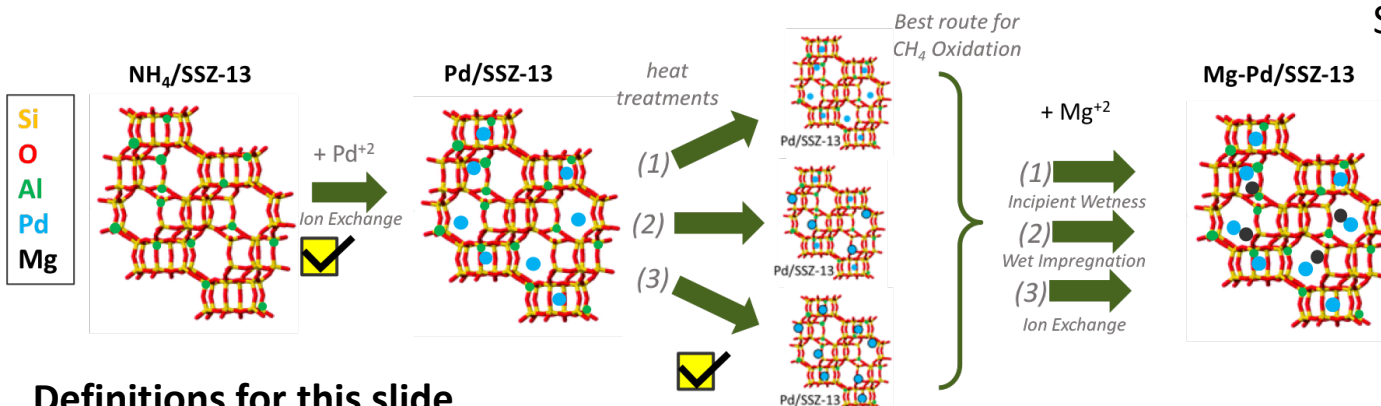
All data and images on this page is covered under the following patents:  
US9353674, JP6383820

MCE: Multi-cylinder engine



# Technical Accomplishments and Progress

Developing new Methane Oxidation Catalyst (MOC) for low temperature CH<sub>4</sub> conversion



Synthetic exhaust composition

	Lean-MOC
	[200 L <sub>flow</sub> /(g <sub>cat</sub> *h)]
H <sub>2</sub> O	12%
O <sub>2</sub>	9%
CO <sub>2</sub>	6%
CH <sub>4</sub>	3000 ppm
CO	2000 ppm
NO	500 ppm
Ar	Balance

## Definitions for this slide

Al: Aluminum

Ar: Argon

cat: Catalyst

CH<sub>4</sub>: Methane

CO: Carbon monoxide

CO<sub>2</sub>: Carbon dioxide

g: Gram

h: Hour

H: Hydrogen (chemical element)

H<sub>2</sub>O: Water

L: Liter

Mg: Magnesium

min: Minute

NH<sub>4</sub>: Ammonium

NO: Nitric oxide

O: Oxygen (chemical element)

O<sub>2</sub>: Oxygen (molecular allotrope)

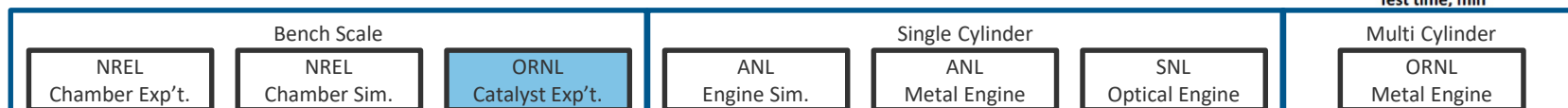
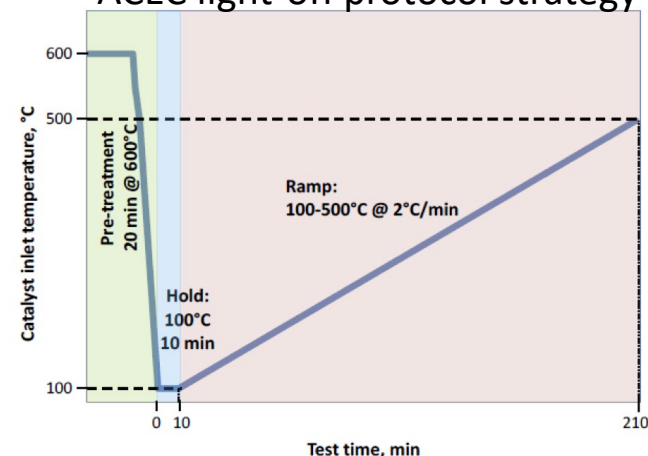
Pd: Palladium

ppm: Parts per million

Si: Silicon

SSZ-13: Aluminosilicate zeolite mineral possessing 0.38 × 0.38 nm micropores

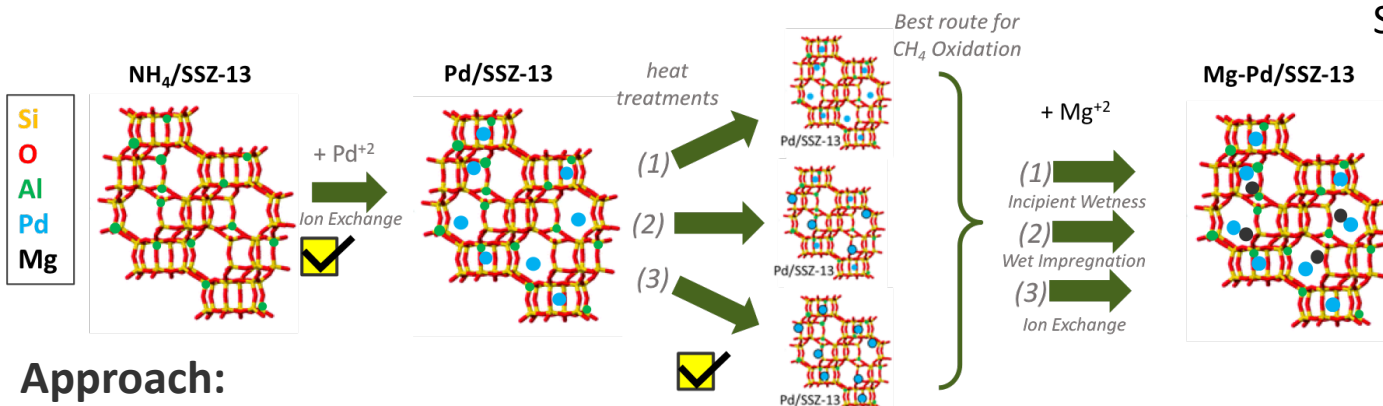
ACEC light-off protocol strategy





# Technical Accomplishments and Progress

Developing new Methane Oxidation Catalyst (MOC) for low temperature CH<sub>4</sub> conversion



Synthetic exhaust composition

	Lean-MOC
	$[200 L_{\text{flow}} / (g_{\text{cat}} \cdot h)]$
H <sub>2</sub> O	12%
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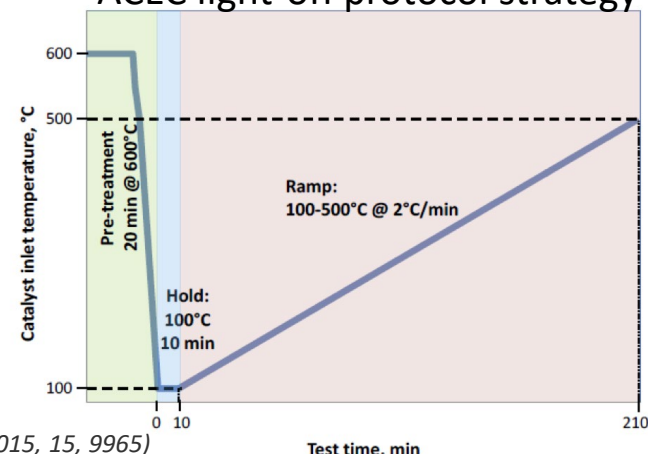
## Approach:

- ORNL synthesized a series of catalysts to lower light-off temperature of methane (CH<sub>4</sub>) oxidation
  - modifying the Pd active site to promote H abstraction using Mg

## Accomplishments:

- Completed synthesis of Pd/SSZ-13 and Mg /SSZ-13
- Examined multiple calcination and hydrothermal treatments
- Evaluated MOCs on a gas flow reactor using a synthetic exhaust flow for a lean natural gas engine
  - Followed U.S. DRIVE (ACEC) catalyst protocol

ACEC light-off protocol strategy



Modified base Si-O chabazite cage structure from (Martin, N.; Moliner, M.; Corm, A. Chem. Commun., 2015, 15, 9965)

Bench Scale			Single Cylinder			Multi Cylinder
NREL Chamber Exp't.	NREL Chamber Sim.	ORNL Catalyst Exp't.	ANL Engine Sim.	ANL Metal Engine	SNL Optical Engine	ORNL Metal Engine

# Responses to Previous Year Reviewers' Comments

This project has not previously been reviewed at a VTO Annual Merit Review.

# Collaboration and Coordination

- **ANL / NREL / ORNL / SNL** collaboration
  - Integrated team of leading experts
  - Hold semi-monthly research coordination and data exchange meetings
- **ANL**
  - Doug Longman (PI)
  - Riccardo Scarcelli
  - Sibendu Som
  - Ashish Shah
  - Joohan Kim
  - Munidhar Biruduganti
- **ORNL**
  - Scott Curran (PI)
  - Josh Pihl
  - Jim Szybist
  - Melanie DeBusk
  - Sreshtha Sinha Majumdar
- **NREL**
  - Brad Zigler (PI)
  - Matt Ratcliff
  - Mohammad Rahimi (post-doc)
  - Shashank Yellapantula
  - Whitney Collins
  - Jon Luecke
  - Ray Grout
- **SNL**
  - Mark Musculus (PI)
  - Zheming Li (post-doc)
  - Rajavasanth Rajasegar (post-doc)
  - Yoichi Niki (visiting scientist)
  - Dalton Carpenter (2018 intern)

# Collaboration and Coordination

- **Altronic**
  - Supplied NGI-1000 flexible natural gas engine spark ignition system to all four DOE labs to support experiments
- **ASG Analytik-Service Gesellschaft mbH**
  - Integrated revised controls and data acquisition for PCSI module in NREL's Advanced Fuel Ignition Delay Analyzer (AFIDA)
- **MAHLE**
  - Collaborated with ORNL to integrate MAHLE Turbulent Jet Ignition (TJI) PCSI system for DD13 multi-cylinder engine experiments
- **Daimler Trucks North America (Detroit Diesel)**
  - Collaborated with ORNL to provide details for modification and support for DD13 for multi-cylinder engine experiments

# Remaining Challenges and Barriers

While the ANL, NREL, ORNL, and SNL research tasks are highly collaborative and integrated, they are still low TRL in nature...

## B1: Science base

- We are developing a fundamental science base and simulation tools to predict fluid-mechanical and chemical-kinetic processes governing PCSI

## B2: Dilution

- Our conclusions will apply generally to design of PCSI for highly dilute / lean combustion, rather than to specific hardware / strategy optimization

## B3: Pre-ignition

- Although insight will be gained, fully addressing pre-ignition at high loads is outside the scope

## B4: CH<sub>4</sub> catalysts

- We will have bench-scale MOC research, but not full catalyst development or engine integration

Additional research and development is necessary for industry to commercialize high efficiency NG engine based on PCSI.

# Proposed Future Research

For the remainder of this funded project:

- Continued sensitivity studies on PCSI geometry parameters, pre-chamber mixture strength, and ignition performance over a range of EGR and lean main chamber dilution
- CFD simulations and optical engine studies to provide conceptual insight into the ignition processes and characteristics of the turbulent flames / jets
- Integration of the single cylinder studies to multi-cylinder dilution / thermodynamics studies
- Feedback of exhaust characterization to MOC studies

With additional funding, proposed future research\*:

- Integrate newly developed science base and tools to guide PCSI research in conjunction with lean / EGR dilute engine combustion development and new MOC for high efficiency engine demonstration – potential industry partnership

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



# Summary: Fundamental experiments & simulation to improve PCSI MD/HD NG engine systems

- ANL, NREL, ORNL, and SNL are collaborating to identify, understand, and simulate fundamental phenomena that limit pre-chamber spark-ignition (PCSI) system efficiency for MD/HD natural gas engines
- The project uses simulations and coordinated experiments to connect bench-scale and single-cylinder facilities to practical multi-cylinder engine and emissions-control hardware
- To extend the lean/EGR dilution limits and/or shorten the burn duration, modes of jet-ignition and resulting progression of main-chamber combustion must be better understood and then predicted through simulation
- To reduce emissions-control constraints on engine operating conditions, factors controlling methane oxidation must be better understood and new approaches must be developed to extend the low-temperature limits of catalysts
- Initial results have pointed toward unexpected in-cylinder jet-to-jet variability, certain inadequacies of state-of-the art models, and encouraging directions for new methane oxidation catalysts

This project is a collaboration between ANL, NREL, ORNL, and SNL. The project team members wish to thank Kevin Stork and DOE Vehicle Technologies Office for support of this research.

# Thank You

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**[www.nrel.gov](http://www.nrel.gov)**

Publication Number

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# Technical Back-Up Slides

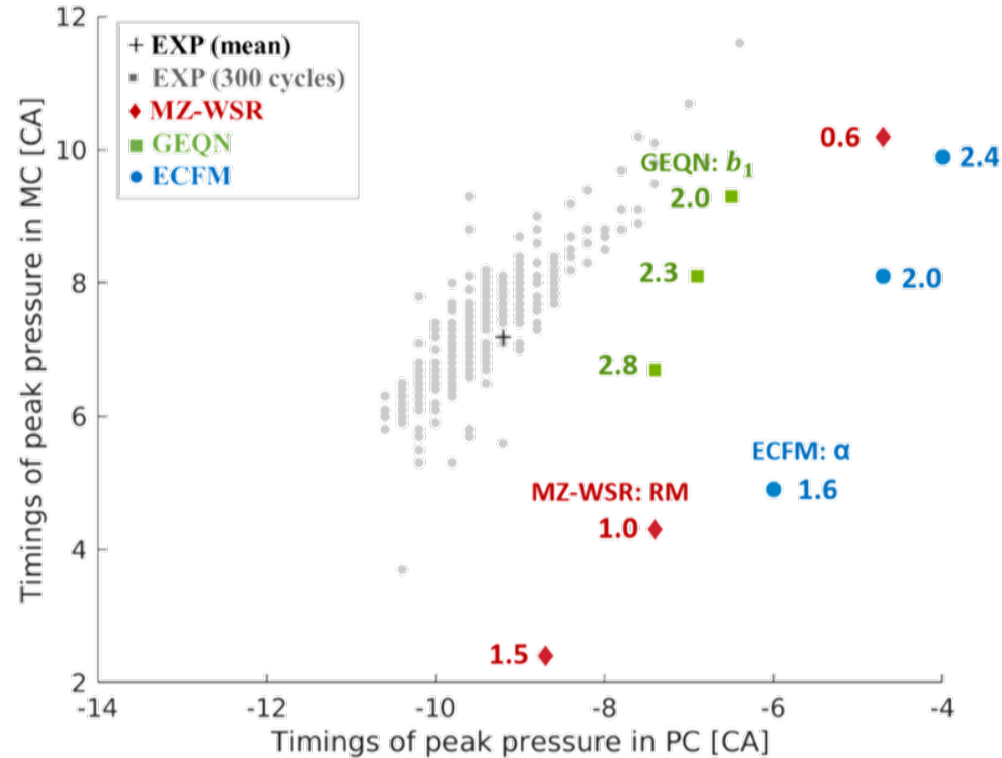
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# Experimental Parameters Across Labs

	ANL	NREL	ORNL	SNL
<b>Engine/Main-Chamber</b>			DD13	
No. cylinders	1	(chamber)	6	1
Displacement [l/cyl]	1.85	0.38 (chamber vol.)	2.13	2.34
Bore [mm]	130	100 (chamber diam.)	132	140
Squish height [mm]	0.8	40 (chamber length)		5.5
Bowl diameter [mm]	100	none (conical P/T and T/C port)		100
Bowl depth [mm]	26	none (conical P/T and T/C port)		15.5
Main-chamber fueling	Fumigation	Mass Flow Controller	Fumigation and/or DI	Fumigation and/or DI
<b>Initial Pre-Chamber</b>			MAHLE	
Volume [cc]	4.67	4.5	1.5 – 6.0	5.5 - 8.4
Number of holes	8	8	6,8	8
Hole diameter [mm]	1.6	1.6	1.2-1.5	1.6
Included angle [degrees]	130	130	120	130
Pre-chamber fueling	Check-valve	DI Bosch (Ford GDI part)	DI	DI Bosch (Ford GDI part)
Spark plug	M8 - NGK ER9EHIX	NGK ER9EHIX (Mini Rimfire can also be packaged)	M8 – Denso/NGK	Mini Rimfire
Ignition	Continuous	Cycles are user selectable	Continuous	Skip-fire
<b>Measurements</b>				
Exhaust emissions	Full exhaust gas analysis NO <sub>x</sub> , THC, CH <sub>4</sub> , CO, CO <sub>2</sub> , O <sub>2</sub> , and CO <sub>2</sub> (EGR)	NO <sub>x</sub> , CH <sub>4</sub> , CO <sub>2</sub> , CO, O <sub>2</sub> + detailed HC speciation	5 Gas Bench + CH <sub>4</sub> + FTIR (exhaust/ EGR) + advanced speciation /PM as needed	None
Chamber pressures	Main and Pre	Main and Pre	Main and Pre	Main and Pre
Indicated efficiency	Yes	NA	Yes – all 6 cyl	Yes
Brake efficiency	Limited (1-cyl setup)	NA	Yes	No
Optical diagnostics	AVL VisioScope possible with cylinder head modification	No	No	Yes

# Preliminary evaluation of combustion models

- Conventional model tuning was not effective for PCSI simulation
  - Experimental data for all cycles showed a good correlation between timings for  $p_{(max, PC)}$  and  $p_{(max, MC)}$ , which implies later jet exit will have lower peak pressure.
  - However, despite typical model tuning efforts, all models kept showing an offset to experiments.
  - G-Equation model offered the opportunity to tune the small scale turbulence constant.



Model	Tunable constant	Description
MZ-WSR	Reaction multiplier (RM)	Modify the chemical reaction rate
GEQN	$b_1, b_3$	Large scale turbulence, $s_t - s_L \sim b_1 u'$ Small scale turbulence, $\frac{s_t - s_L}{s_L} \sim b_3 \left(\frac{D_t}{D}\right)^{1/2}$
ECFM	$\alpha, \beta$	Flame stretch as source, $P = \alpha K_t f(u', l, s_L, l_f)$ Flame destruction as sink, $D = \beta s_L \frac{\Sigma^2}{1 - \tilde{c}}$