SAND2020-4474PE

Medium-Duty Diesel Combustion

Project ID: ace136

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Sandia National Laboratories

2020 DOE VTO Annual Merit Review

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Overview

Timeline

- December 2017-present: medium-duty diesel research
- Ongoing project with continual guidance from AEC MOU industrial partners and reviewers

Barriers & technical targets

- Lack of quantitative engine combustion databases precludes collaborative model verification and validation
- Inadequate understanding of fuel injection, air motion, and combustion chamber geometry effects on combustion and pollutant formation
- Research priorities for MCCI:
  - Reduced engine-out NOx and particulates
  - Reduced cold-start emissions

Budget

FY19: $900k
FY20: $850k

Partners

Ford: Technical/engineering support, regular meetings and teleconferences

WERC – Wisconsin Engine Research Consultants: RANS 3D-CFD simulations; Model development and evaluation

Relevance and current objectives

Relevance

- Improving MCCI combustion system efficiency and emissions behavior will require improved understanding of how spray-wall interactions can promote rapid fuel-air mixing
- Clean catalyst heating operation is critical to enable fuel efficient diesel engines to comply with new CARB regulations (e.g. 0.02 g/bhp-hr NOx)

Objectives for this period

- Commission new, medium-duty diesel research engine and all auxiliary systems
- Bowl geometry study
  - Develop tools needed to design and optimize a DSL piston for the new engine
    - Novel, physics-based optimization metric
    - Fully parameterized DSL piston design to enable optimization
    - 1D GT-Power model to aid CFD simulations
    - 3D mesh for CFD simulations of flow, mixing, and combustion — WERC Wisconsin Engine Research Consultants
- Catalyst heating operation study
  - Analyze high-speed imaging data to provide insight into sources of UHCs
  - Perform initial experimental studies (delayed)
  - Develop CFD models to predict mixture formation and combustion of late post injections during catalyst heating operation
  - Provide insight into cetane number effects

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CRF

Milestones

FY20

- Q1: Complete shakedown testing of new medium-duty diesel engine **In progress/ delayed**
- Q3: Tradeoffs between pollutant emissions and exhaust temperature/heat flux in catalyst heating operation **Likely delayed**

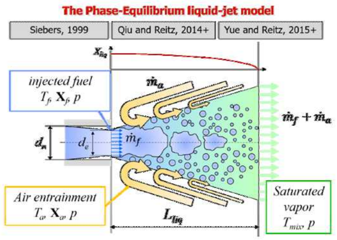
FY21

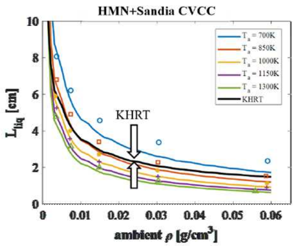
- Q1: guidance for use of phase-equilibrium liquid jet modeling approach for catalyst heating operation
- Q3: experimental characterization with DSL piston; test hypothesis that improved vortex formation can improve efficiency and/or reduce pollutant emissions

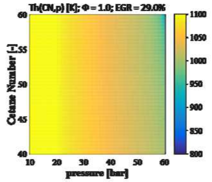
Approach: catalyst heating operation

Experiments provide insight into mixture formation and combustion; they are used to develop and evaluate novel approaches to CFD spray modeling

CFD simulations and analyses







Critical ignition temperature is less sensitive to cetane number for late post injections

2019

Begin developing phase equilibrium model

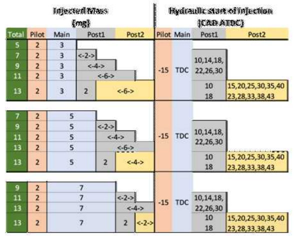
Develop injection strategies; initial performance/emissions testing

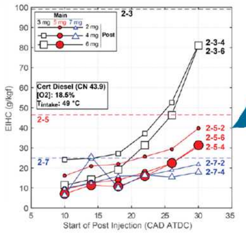
2020

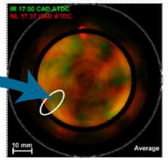
Implement phase equilibrium model; evaluate using ECN Spray A and small-bore engine data

High-speed NL and IR imaging and analysis

Develop catalyst heating operating mode in medium-duty engine. Improve understanding of mixture preparation and pollutant formation processes; develop science-based guidance for cat heating operation.







Evidence pilot + main may be a significant source of UHC emissions

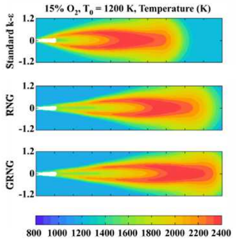
New engine

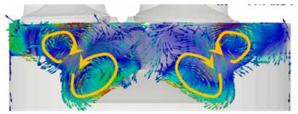
Thermodynamic / optical experiments and analyses

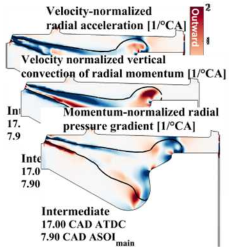
Approach: piston bowl geometry study

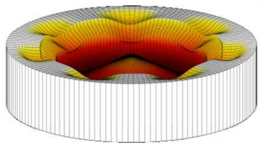
Utilize thermodynamic / optical experiments and in-depth analyses of 3D CFD results to develop and test a hypothesis: enhancing vortex formation will increase efficiency and reduce emissions

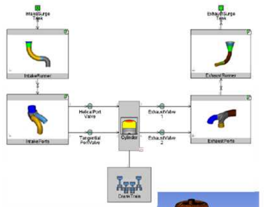
CFD simulations and analyses

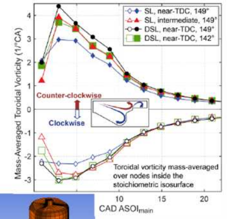


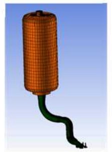


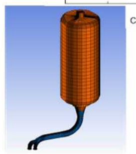




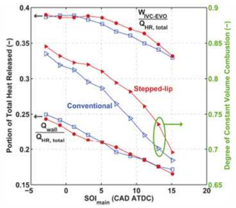


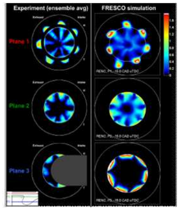


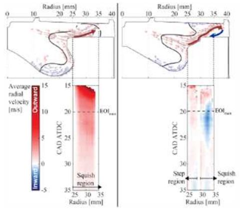




2016	2017	2018	2019	2020	
Model evaluation, description of flow evolution	Develop CFD simulation analysis tools	Spray-wall dynamics analysis, parametric study	Dimpled stepped-lip (DSL) piston hypothesis	Develop models & metric to optimize DSL piston	CFD optimization of DSL geometry for new medium-duty diesel engine; validation through engine experiments
Engine experiments; compare two piston bowl designs	Fuel vapor fluorescence imaging	High-speed optical characterization of flow evolution	Develop new medium-duty diesel engine	Commission medium-duty diesel engine	





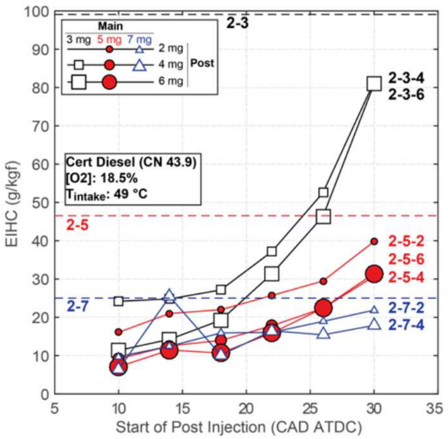


Thermodynamic / optical experiments and analyses

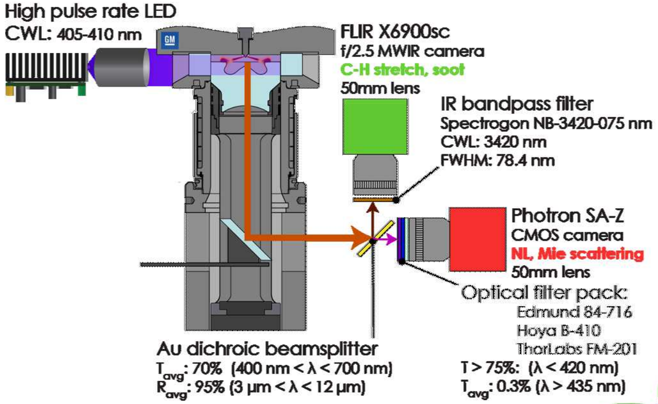
TA: high-speed imaging results support the hypothesis that pilot and main mixture may be a significant source of UHCs in cat heating operation

- Analysis of high-speed imaging in the small-bore engine provides initial insight into mixture formation, combustion, and pollutant formation in catalyst heating operation
- 2019 results: adding a small post injection reduces UHC emissions, regardless of post timing
- 2020 results: **visual evidence that pilot and main injections may be a significant source of UHC emissions**
  - Evidence of incompletely burned pilot/main fuel in the bowl at time of post injection
  - Diminishing interaction between post and bowl contents as post injection is retarded – late posts may be unable to help mixture in the bowl to react to completion

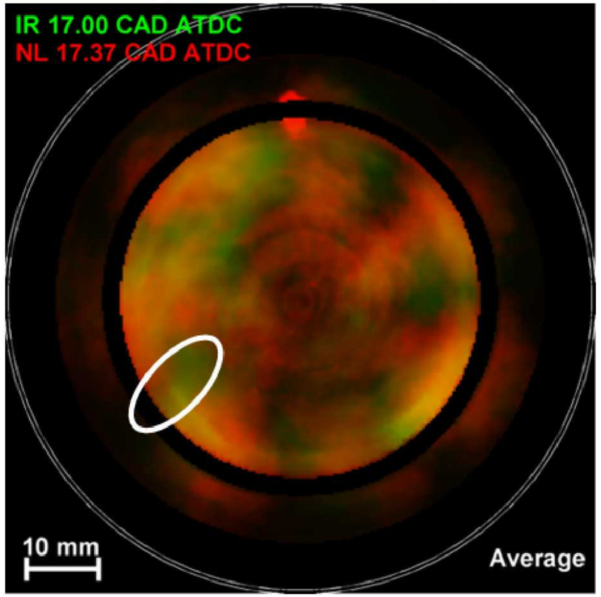
FY19 result: post injections reduce UHCs



FY20: high-speed infrared and visible imaging: insight into mixture formation and combustion

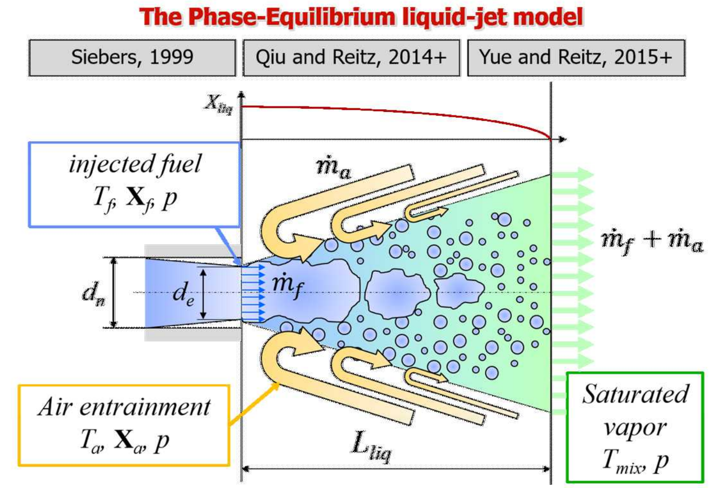


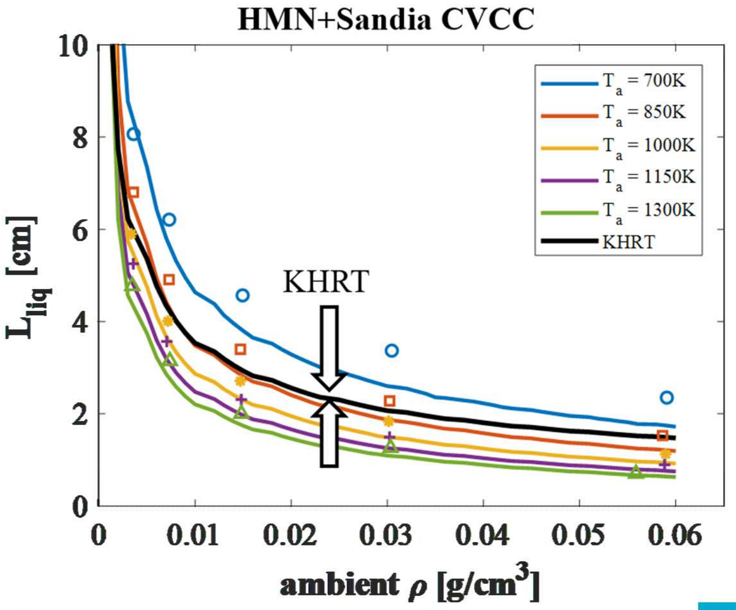
Images taken shortly before late post injection indicate unburned hydrocarbons persist in the bowl



TA: vapor-liquid equilibrium modeling enables prediction of spray behavior into a wider range of in-cylinder conditions

- State-of-the-art KH-RT Spray breakup models are predictive only over a limited range of in-cylinder conditions
- Catalyst heating operation involves multiple injections into a wide range of in-cylinder temperatures and pressures – an improved modeling approach is needed
- The vapor-liquid phase equilibrium model and a real-gas equation-of-state have been implemented in the FRESCO code
- **3D CFD simulations are now capable of prediction of spray behavior over a wider range of temperatures and pressures**





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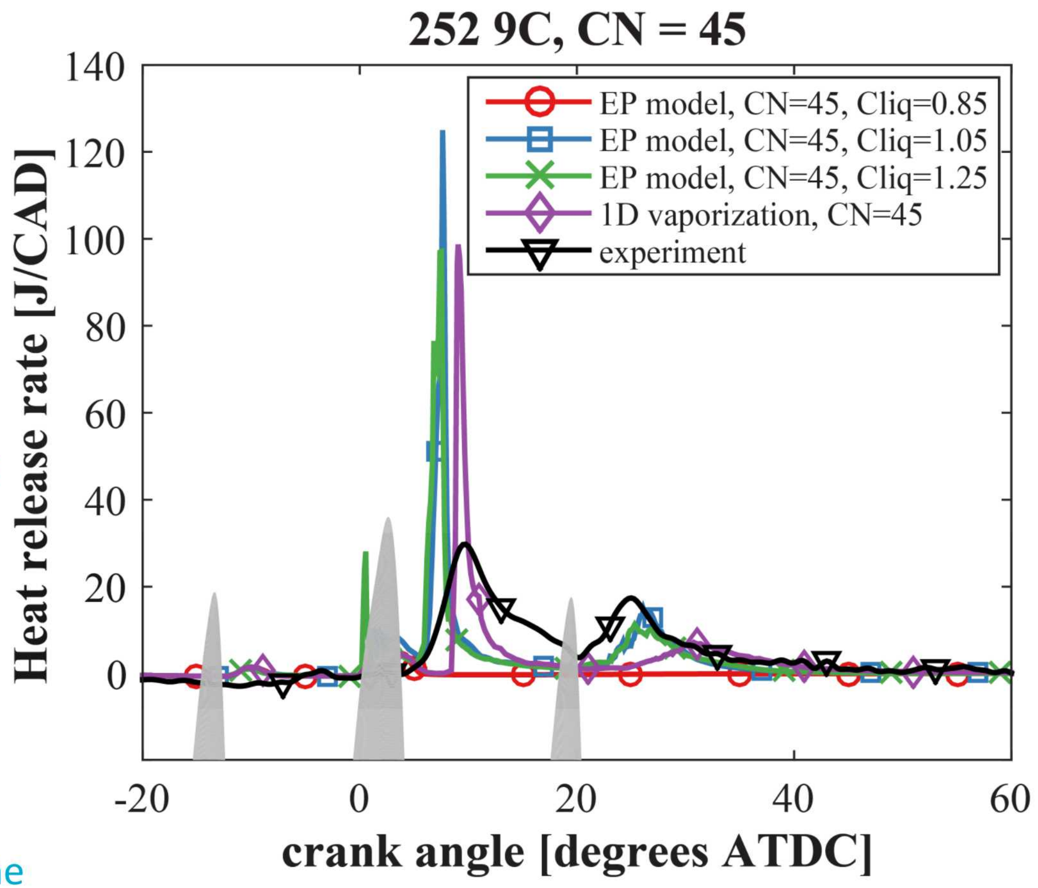
Update: phase-equilibrium model can improve prediction of post injection heat release

- Latest FRESCO simulation results: pilot-main-post injection strategy, primary diesel reference fuels; sector mesh
- Ignition of pilot, main, and post injections is extremely sensitive to cetane number and spray/mixing predictions
- Pilot and main heat release rates are over predicted
  - Possible reason: lower turbulence levels inherent in sector-mesh simulations
  - Investigations into this behavior continue
- **Post-injection ignition can be better predicted with the phase-equilibrium model; most significant difference in results is the predicted liquid length**
  - This modeling approach is being evaluated/tuned with available optical engine data and will be applied to predict catalyst heating operation in the new engine



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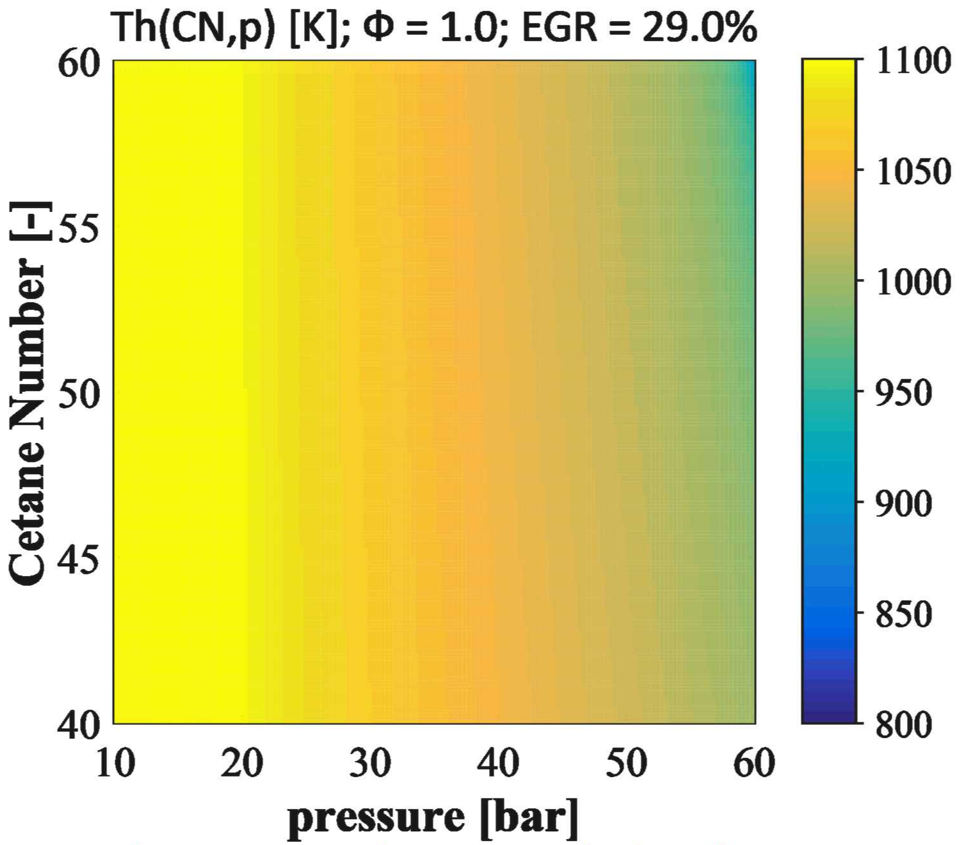
TA: kinetic simulations provide insight into the role of cetane number in the ignition of late posts

- 0D kinetic study utilized a stoichiometric mixture of the diesel primary reference fuels (n-hexadecane and 2,2,4,4,6,8,8-heptamethylnonane)

- Minimum ignition temperature (T_h) is defined: high-temperature ignition will occur within 4 CAD at 1500 rpm (~440 µs)

- Ignition delay becomes less sensitive to cetane number as post injections are retarded and cylinder pressure decreases; this finding is largely independent of equivalence ratio and EGR rate

- **Implication: the mechanism by which increased cetane number improves post injection retardability[1] likely depends more on the successful ignition of the pilot and main to increase T, P**



As pressure decreases during the expansion stroke, increasing cetane number may not directly help post injections ignite

[1] Kurtz, E. and Polonowski, C., "The Influence of Fuel Cetane Number on Catalyst Light-Off Operation in a Modern Diesel Engine," SAE Int. J. Fuels Lubr. 10(3):2017, https://doi.org/10.4271/2017-01-9378.

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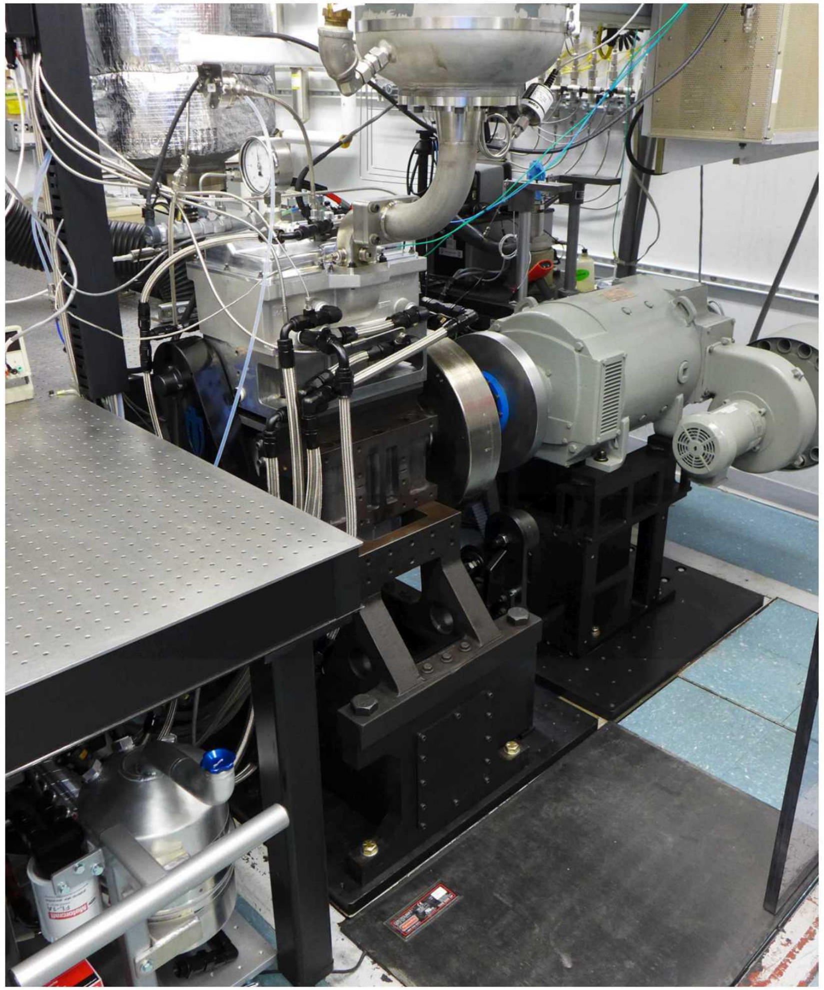
WERC

TA: the new medium-duty diesel engine and all auxiliary systems have been successfully commissioned

- Dual configuration: all-metal (FY20) and optical (in design)
- Planned experiments
  - Testing the DSL piston hypothesis with a CFD-optimized piston (see future work slide for details)
  - Continued catalyst heating studies: developing understanding of pollutant formation mechanisms and keys to post injection retardability

Bore	99 mm
Stroke	108 mm
Compression ratio	16.2:1
Valves/cylinder	4
Injector	8-hole piezo
Piston bowl shape	Stepped-lip (Ford 6.7L)
Max speed	2000 rpm
Max rail pressure	2000 bar
Lubrication system	Dry sump

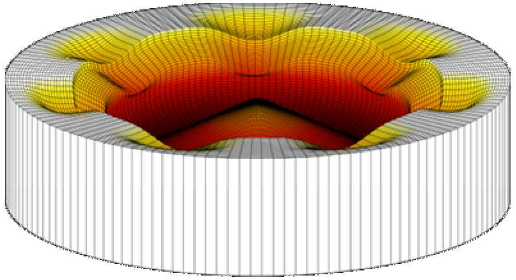


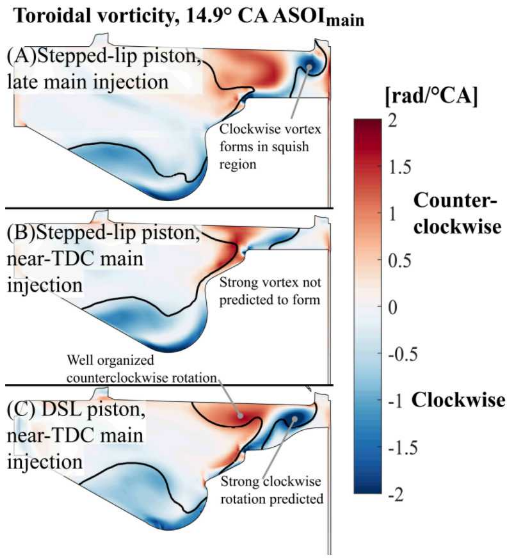
Ford is gratefully acknowledged for providing the short block and other critical hardware, and for significant engineering support

TA: a novel metric has been developed to facilitate DSL piston optimization

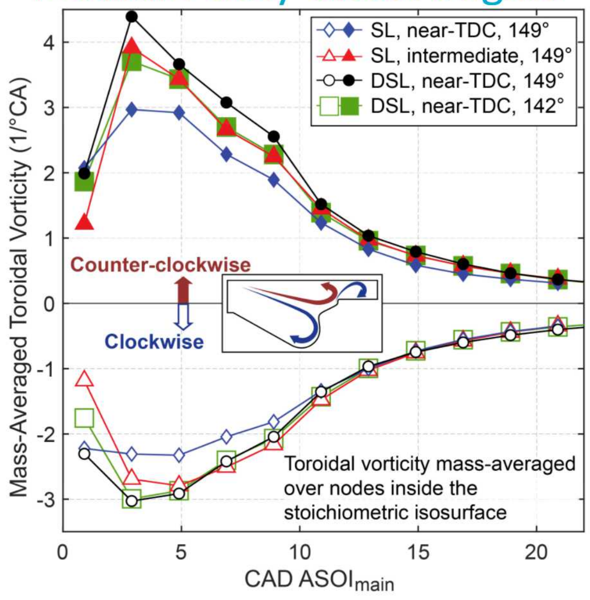
- A quantitative measure of vortex strength is needed for CFD-based design and optimization of a DSL piston to test the hypothesis: stronger, longer lived vortices will improve efficiency and reduce emissions
- 2019 results: the DSL piston promotes vortex formation at near-TDC injection timings
- 2020 results: **toroidal vorticity, mass averaged inside the stoichiometric isosurface, captures the sensitivity of predicted vortex strength to injection timing and bowl geometry**
  - This new metric will be used to develop a DSL piston for the medium-duty diesel engine

FY19 result: DSL piston promotes vortex formation[2]





FY20: a novel metric has been created that will enable optimization of a DSL piston design for the medium-duty diesel engine

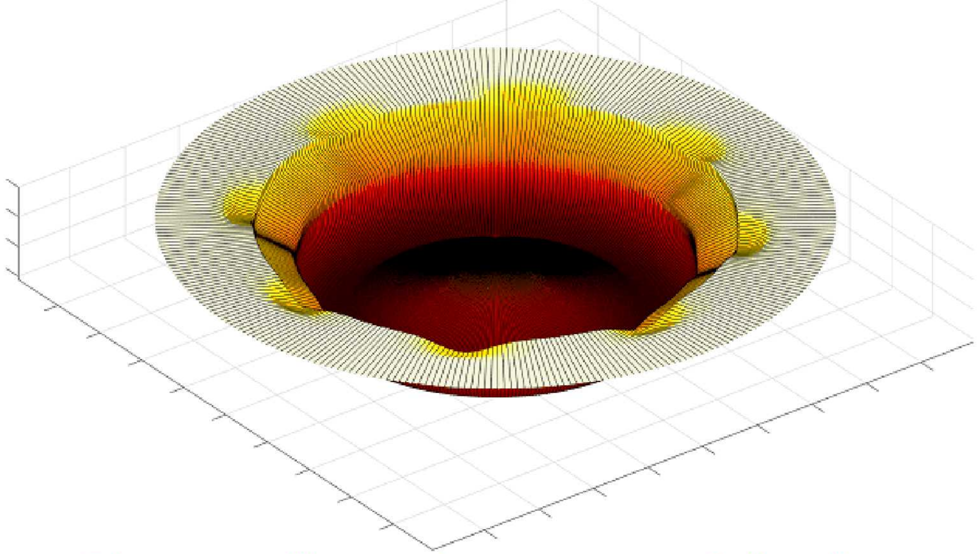


[2]Busch, S., Perini, F., Reitz, R., and Kurtz, E., "Effects of Stepped-Lip Combustion System Design and Operating Parameters on Turbulent Flow Evolution in a Diesel Engine," *SAE Int. J. Engines* 13(2):2020.

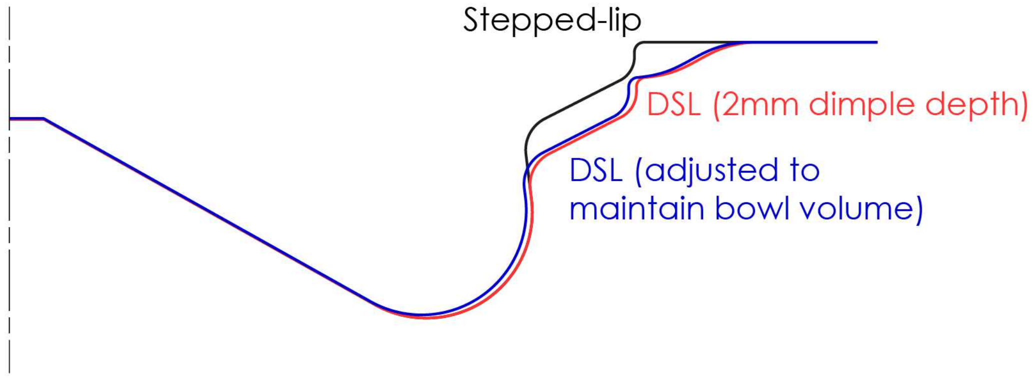
TA: DSL piston design has been fully parameterized for optimization work

- DSL piston optimization must be performed with a constant compression ratio
- For a given set of DSL geometric parameters (dimple depth, width, radial extent), the bowl must be scaled to maintain a constant volume
- The production piston geometry has been fully parameterized and automated adjustment of bowl size maintains bowl volume within ~0.025% of the baseline
- Additional finding: for fixed bowl volume, DSL pistons have a lower surface area/bowl volume ratio than the stepped-lip piston
    - As shown at right: ~0.8% reduction compared to production piston
    - Increased wall heat losses are not expected with DSL pistons

Volume-corrected DSL piston with 8 dimples



Piston profiles at deepest part of dimple



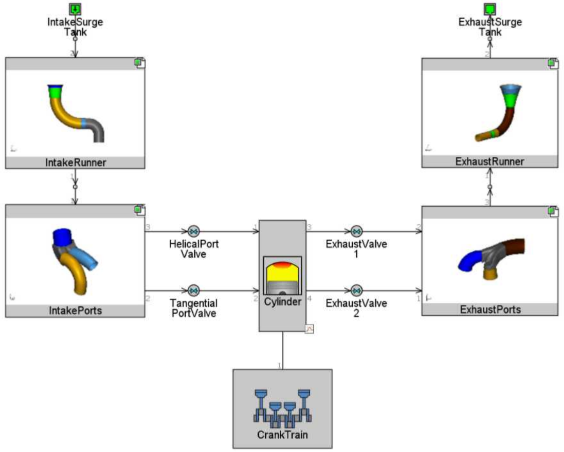
Update: developing and characterizing catalyst heating operation in the new engine

- Progress in the lab has been halted by the COVID-19 pandemic
- **Experiment preparation / engine operation will resume as soon as possible**

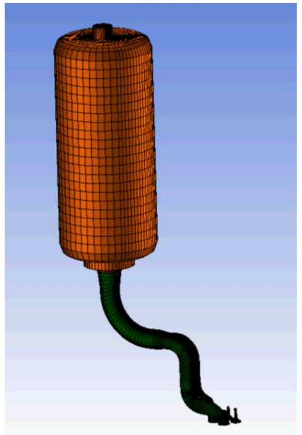
Update: 1D GT-Power model and 3D mesh have been created for the new medium-duty diesel engine

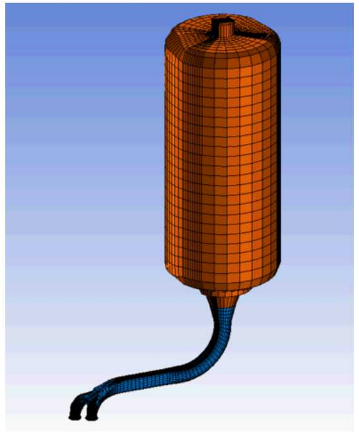
- Progress on 1D GT-Power model
  - 1D simulations are needed for accurate boundary/initial conditions for 3D CFD studies
  - SNL: 1D model (GT-Power) is complete; model tuning and validation will commence as engine measurement data become available
- Progress on 3D CFD simulation efforts
  - W-ERC: 3D meshing of intake, cylinder head/combustion chamber, and exhaust systems is ongoing
  - SNL: The FRESCO CFD solver is being installed on Sandia's computing cluster
  - New post-doc starts in June to work on bowl geometry study

GT-Power model derived from CAD geometry



3D mesh partially complete (optimization in progress)



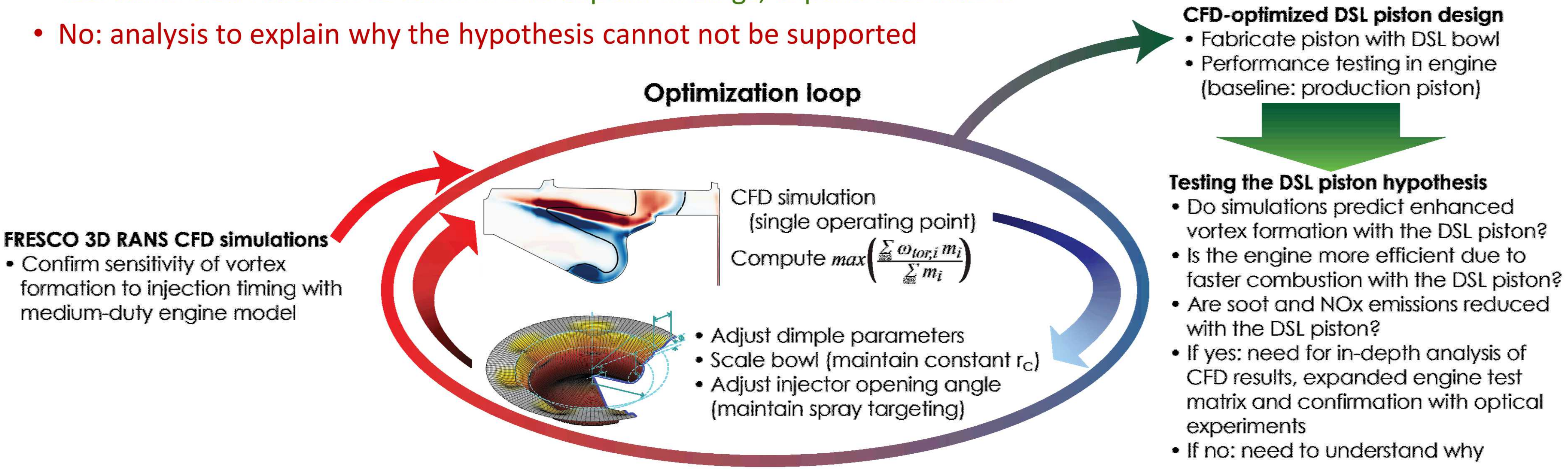


Response to reviewer comments

- CFD simulations of catalyst heating may help identify sources of UHCs and combustion inefficiency
    - Accurate, predictive simulation of catalyst heating operation remains challenging and we continue to evaluate our current approach with available optical data. More experimental data will likely be needed to draw conclusions about sources of UHCs.
- Efforts should be made to bring the new research engine online in FY19 and to maintain the research approach
    - Despite many unforeseen yet unavoidable and time-consuming setbacks in the construction and commissioning of the engine, it is finally operational and research continues. Fortunately, parallel efforts to develop simulation capabilities have progressed independently of these setbacks. Our research approach continues to evolve as new understanding is developed but it is fundamentally unchanged.
- Post injections initially decreased particulates, so the following hypothesis was found to be inadequate: late injection targeting cannot create sustained vortices near top-dead-center; further insight is needed
    - There appears to have been some misunderstanding: no particulate emissions data have been shown for the post injection study. The observations of long lived vortices forming for late injection timings, but not for near-TDC injections, was made for conventional diesel operation, not catalyst heating operation with very small injection quantities and including post injections.
- It would be good to connect this work with other work at Sandia and in the ECN to share the learning from this project and develop other experiments to provide further insight
    - There is a need for better fundamental understanding. We continue to engage in discussions with other researchers with the limited time and resources available; it is difficult to align the experimental objectives of different projects with different missions.
- Too few details are provided to demonstrate how this study will achieve its scientific objectives
    - Last year's poster did not provide adequate detail about the methodologies that are being developed and applied to achieve project objectives. The remaining slides should help address these concerns.

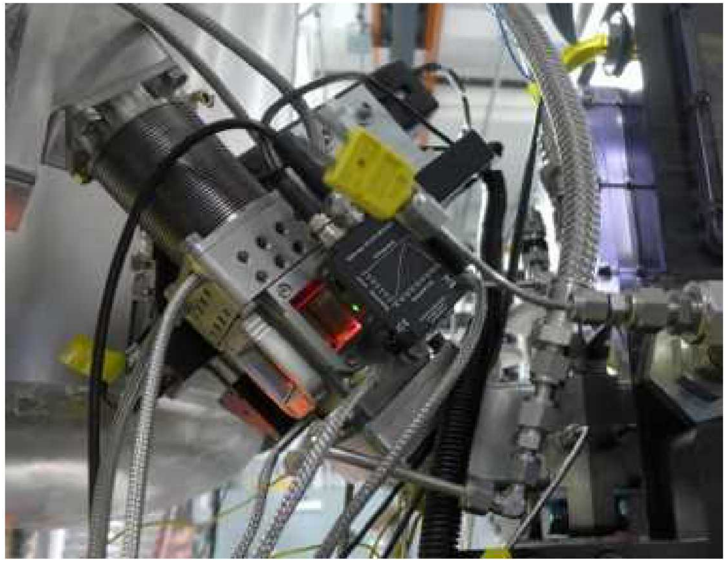
Remaining challenges / future research: piston geometry study

- Observed strength/longevity of vortices correlates with faster, cleaner, more efficient combustion
- CFD simulations qualitatively predict the experimentally observed vortex behavior in the squish region
- Use validated CFD approach to develop an optimized DSL piston
- Results of engine performance testing: can the DSL piston hypothesis be supported?
    - Yes: continued research to confirm and explain findings; expand test matrix
    - No: analysis to explain why the hypothesis cannot not be supported



Remaining challenges / future research: catalyst heating study

- **Challenge:** Emissions of unburned hydrocarbons (UHC), including formaldehyde (CH2O), remain as a barrier to effective catalyst heating operation
- **Objective:** improve fundamental understanding of origins of UHC and CH2O formation
- **FY21 plans**
  - Continue design and fabrication of optical engine
  - Develop and apply technique to provide time-resolved measure of UHC / CH2O / soot in the exhaust runner
    - Adapt fast runner extinction diagnostic (FRED) system (originally developed by Chuck Mueller / Nathan Harry, SNL) to medium-duty diesel engine
    - Implement multiple wavelengths for online/offline CH2O measurement
    - Time-resolved measurement of UHCs/CH2O, combined with CFD simulations, is expected to provide insight into the spatial origins of these pollutants based on its behavior during the exhaust stroke



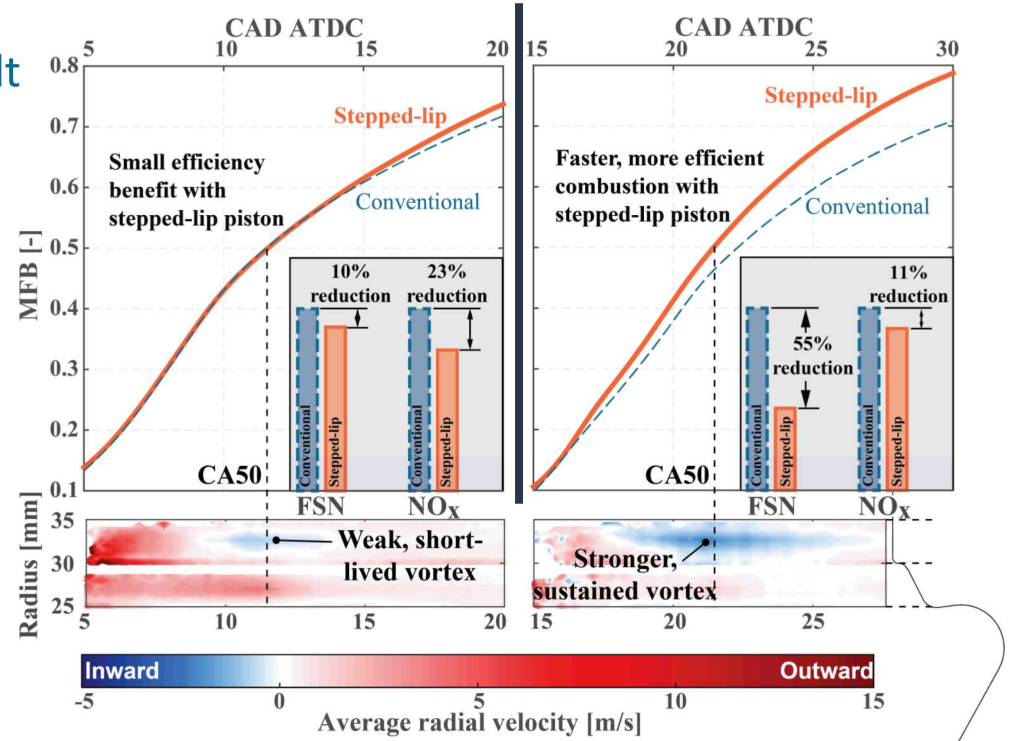
Thank you for your attention

Your questions and feedback are welcome

Technical Backup Slides

Experimental support for the DSL piston hypothesis

FY18 result



Near-TDC injection

- Small difference in rate of mixing controlled heat-release
- Modest soot reduction
- Weak vortex in squish region

Late injection

- Faster, more efficient combustion
- Substantial soot reduction
- Stronger, longer-lived squish region vortex

Observation: faster, more efficient mixing-controlled heat-release rates correlate with stronger vortex action.

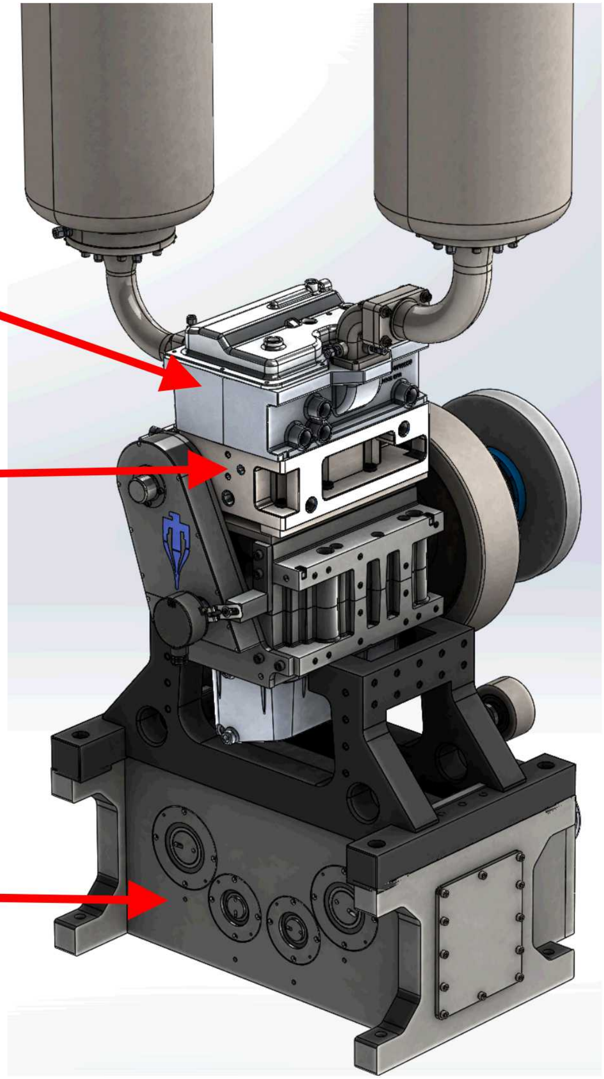
Hypothesis: promoting vortex formation at near-TDC injection timings may improve peak efficiency and reduce emissions.

Sandia's Medium-Duty Diesel Engine

Cast aluminum cylinder head

Custom deck adapter facilitates conversion to optical engine

Reconfigurable, belt-driven Lanchester balancing box (1^{st} and 2^{nd} order)



Sandia’s Medium-Duty Diesel Engine

Adjustable exhaust back pressure

Control of intake flow rate, composition, and temperature

Measurement of coolant temperatures and flow rates

Dry sump lubrication system with electrically driven, five-stage pump

Engine after dry-fit test