I.1 Diesel Combustion for Medium-Duty Off-Road Applications (Sandia)

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Project Introduction

Rapid fuel/air mixing can reduce fuel consumption and pollutant emissions from diesel engines. In medium-duty diesel engines, interactions between the fuel sprays and the piston bowl walls play a key role in determining mixing-controlled heat-release rates. Stepped-lip pistons can promote the formation of vortices that are correlated with faster, more efficient heat-release and reduced soot emissions, but this behavior is primarily observed for late injection timings at which the engine is not operating at its peak efficiency [1]. Activity in this fiscal year is directed at dimpled stepped-lip (DSL) pistons, which are predicted to promote robust vortex formation. Computational fluid dynamics (CFD) simulations quantify the effects of the dimples on rotational energy and engine experiments quantify the DSL piston's effects on efficiency.

Diesel exhaust-aftertreatment systems effectively eliminate pollutants such as carbon monoxide, nitrogen oxides, and unburned hydrocarbons, but only after catalysts have been warmed to their light-off temperatures of approximately 200°C. The goal of engine operation during the first minutes after a cold start is to quickly heat up the exhaust aftertreatment system while minimizing untreated pollutants. This task is most challenging when the engine is idled or operated at low loads. Catalyst heating operation involves multiple injections spanning a wide range of crank angles and thermodynamic states of the in-cylinder gas, with the intention of increasing exhaust temperature/enthalpy. Incomplete combustion results in tradeoffs between exhaust enthalpy, pollutant emissions, and fuel consumption [2], which have been studied through experiments in Sandia's off-road diesel research engine. The effects of varying fuel reactivity on this operation have also been investigated and thermodynamic analyses provide insight into how this property can affect the engine's catalyst-heating performance.

Objectives

This project will provide scientific understanding needed to design, optimize, and calibrate the next generations of off-road diesel engines that comply with increasingly stringent pollutant emission regulations while achieving thermal efficiencies exceeding 50%.

Overall Objective

- Develop conceptual models for spray-wall interactions, combustion, and pollutant formation in direct-injection diesel engines.
- Provide scientific understanding of aspects of combustion chamber design that enable improvements in efficiency and/or reductions in pollutant emissions.

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- Develop conceptual models that describe fuel injection, mixture formation, combustion, and pollutant formation during catalyst heating operation.

Fiscal Year 2021 Objectives

- Quantify the emissions and efficiency benefits of a baseline DSL piston through engine experiments.
- Perform CFD simulations and analyze the results to provide guidance for DSL geometric parameters and identify an improved DSL geometry that will more effectively promote vortex formation.
- Characterize and explain tradeoffs in catalyst-heating performance over a wide range of injection strategy calibrations and exhaust gas recirculation levels.

Approach

The world's first dimpled stepped-lip piston has been designed in a MATLAB environment and machined from an aluminum piston blank. As discussed in the previous year's report, the bowl dimensions are scaled to maintain a constant volume, such that the engine's compression ratio is unaffected by the addition of the dimples [3]. The DSL piston's effects on efficiency and emissions are evaluated through experiments in Sandia's off-road diesel research engine. Thermodynamic analyses reveal the extent to which the DSL piston enhances mixing-controlled heat release and thermal efficiency compared to operation with the baseline stepped-lip piston.

CFD simulations are performed together with the support of Wisconsin Engine Research Consultants using their FRESCO CFD solver. Metrics are developed to quantify the rotational energy that develops in the squish region of the combustion chamber as a result of interactions between the fuel sprays and the bowl geometry. Simulations are performed with a systematic variation of parameters that affect the dimples' geometry. The rotational energy metric provides directional guidance for a DSL piston variant that is expected to produce significantly more rotational energy.

The space-filling statistical experiment design and experimental methodology developed last year is applied to study catalyst-heating operation in the off-road diesel research engine. Thermodynamic analyses provide insight into the tradeoffs in catalyst-heating performance and pollutant emissions that result from changes in injection strategy calibration and exhaust gas recirculation (EGR). Additionally, the fuel is doped with several different concentrations of a cetane improver to investigate the effects of fuel reactivity on these tradeoffs through additional experiments.

Results

The following key accomplishments for Fiscal Year 21 are reported:

- The baseline DSL piston provides a 1.4% increase in thermal efficiency for a part-load operating point due to faster mixing-controlled heat release.
- CFD simulations have identified an alternate set of geometric parameters for a DSL bowl that result in 44% more peak rotational energy in the squish region than for the baseline DSL geometry.
- Engine experiments provide a clearer understanding of tradeoffs in catalyst-heating performance and pollutant emissions. Analyses identify a mechanism by which increased fuel reactivity can reduce exhaust temperatures, under some circumstances.

To evaluate the benefits of the baseline DSL piston, the engine is operated at part-load at 1600 rpm. This point represents a significant portion of engine operation during typical on-road drive cycles for both conventional and hybrid powertrains. A sweep of main injection timing with the stepped-lip (SL) piston serves as the reference case against which the DSL's benefits are measured. At each injection timing, the following are computed:

1. Thermal efficiency: the ratio of indicated work done in the closed portion of the cycle to the amount of fuel energy released.
2. The (estimated) proportion of released fuel energy that is transferred to the coolant through the combustion chamber walls.
3. The degree of constant volume combustion (dCVC), a measure of how much the combustion event resembles constant-volume combustion.

Figure I.1-1 shows these comparison metrics plotted against the commanded start of the main injection. The DSL piston typically reduces wall heat-loss. This is largely explained by the fact that the DSL piston's surface area is approximately 2.4% smaller than that of the SL piston (see [3]). The dCVC plots (shown with dashed lines) indicate that the DSL piston results in faster combustion for the most advanced (closest to TDC) main injection timings. This faster combustion results in higher thermal efficiency, and the benefits decrease more rapidly with the DSL piston as injection timing is retarded. At the most advanced injection timing, this is a 1.4% relative gain in efficiency. This finding supports the hypothesis developed through prior research (see [4]) that a DSL piston can promote faster combustion and therefore increase efficiency. The first experiments with the DSL piston indicated that it increases smoke emissions at these more efficient injection timings. Ongoing research is focused on understanding this behavior and how this detrimental effect may be avoided.

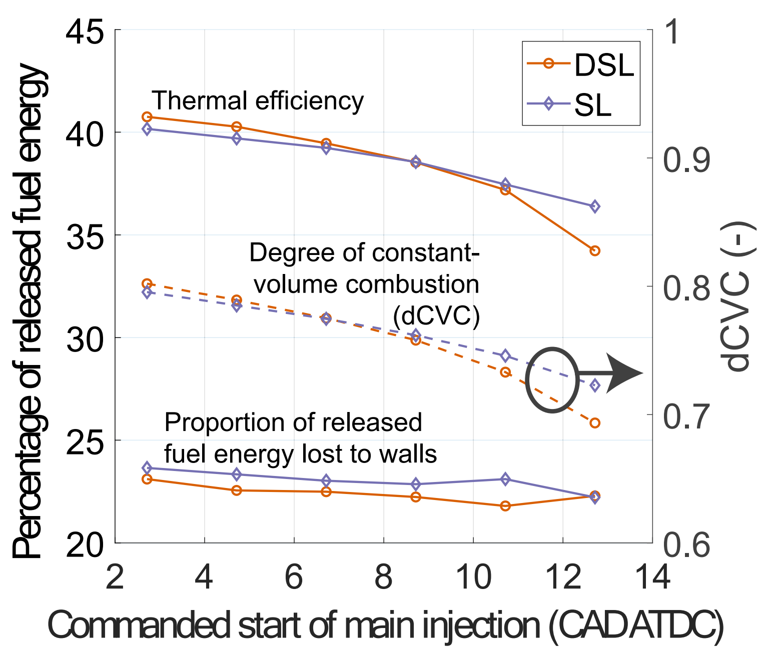


Figure I.1-1: Thermal efficiency, the degree of constant-volume combustion, the proportion of released fuel energy lost as heat through the combustion chamber surfaces as a function of injection timing. The DSL piston improves thermal efficiency for main injections starting near TDC because it results in faster combustion at those injection timings.

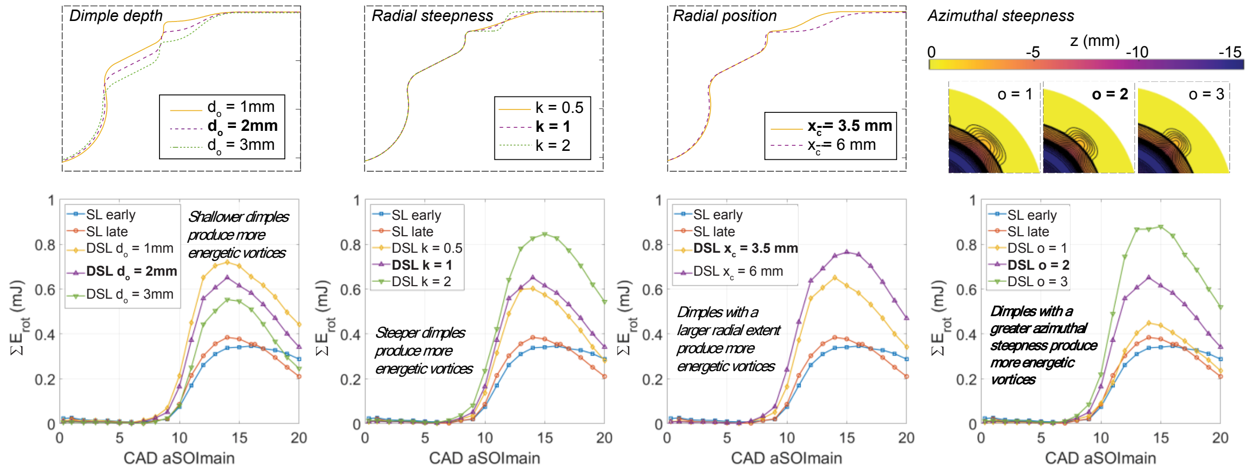
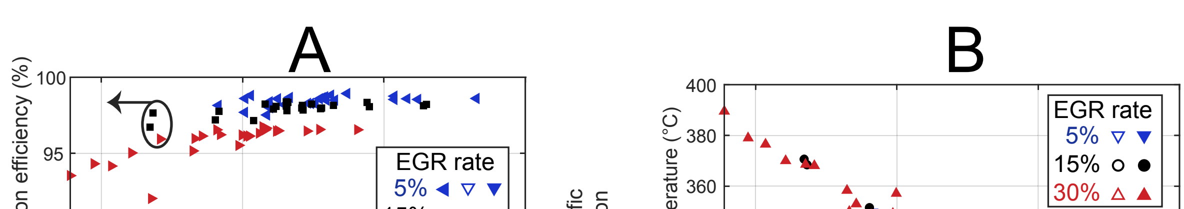


Figure I.1-2: The effects of four DSL geometric parameters (dimple depth, radial steepness, radial position, and azimuthal) are investigated with CFD simulations. The most energetic vortices are produced with shallow dimples with step sides that are located closer to the cylinder wall. The baseline value of each parameter is indicated with bold text.

Computational investigations are performed with a controlled set of DSL pistons designs to provide understanding of how dimple geometry affects flow structures believed to promote faster fuel/air mixing. Figure I.1-2 shows the parameters that have been independently varied and their effect on rotational energy associated with vortices that form in the outer portion of the combustion chamber as the outwardly penetrating fuel sprays interact with the piston walls. Previous investigations in the optical research engine indicated that stronger, longer-lived vortices in this outer region correlate with faster, more efficient combustion [5]. The results shown in Figure I.1-2 provide clear directional guidance for each parameter. The values that yield the highest predicted rotational energies are a dimple depth of 1 mm, a radial steepness factor of 2, a radial position of 6 mm, and an azimuthal steepness parameter of 3. A follow-on simulation with this set of parameters indicates that these effects are synergistic and increase peak rotational energy values by 44% compared to the baseline DSL design. A DSL piston has been produced with these parameters and upcoming engine experiments will evaluate the simulations' ability to provide directional design guidance and whether efficiency can be further improved. Furthermore, both experiments and CFD simulations will focus on the effects of DSL pistons on pollutant emissions.

The experimental approach developed last year (see [2]) to study catalyst-heating operation has been implemented to provide insight into the fundamental tradeoffs between efficiency, exhaust heat, and pollutant emissions. These results are shown in Figure I.1-3; thermal efficiency, indicated specific fuel consumption, combustion efficiency, exhaust temperature, and exhaust heat flux are plotted against the degree of constant-volume combustion. Each point corresponds to a specific injection strategy calibration and the symbols correspond to three different EGR levels. Changes in thermal efficiency, fuel consumption, and exhaust temperature are well explained by changes in the degree of constant-volume combustion. Injection strategy calibrations that result in earlier combustion phasing are more efficient: a greater fraction of the fuel's energy is used to do work, so less energy is available as exhaust enthalpy, and exhaust temperature decreases. As dCVC decreases and as EGR rate increases, emissions of carbon monoxide and unburned hydrocarbons increase, so combustion efficiency decreases. This is associated with the non-linear behavior observed in the fuel consumption data; reducing pollutant emissions is one potential means to improved catalyst-heating strategies. Because the exhaust temperature data collapse well into a single line when plotted against dCVC, increasing EGR likely increases exhaust temperature by shifting the heat-release toward later crank angles. Although the highest exhaust temperatures are achieved at the 30% EGR level, the highest heat flux (enthalpy

Figure I.1-3: A: Combustion efficiency, specific fuel consumption, and thermal efficiency plotted against the degree of constant volume combustion as injection strategy calibration and EGR rate are varied. B: Exhaust temperature and heat flux available for catalyst heating plotted against the degree of constant-volume combustion as injection strategy calibration and EGR rate are varied.



flow rate normalized by engine displacement) is reached at the 5% EGR level. This is because recirculating exhaust gas reduces the flow of mass that would be available to provide heat to the aftertreatment system.

Further catalyst-heating studies are performed to provide understanding of how more reactive (higher cetane rating) fuels can enable hotter exhaust. The baseline certification diesel fuel (CD) is doped with small amounts of di-tert-butyl-peroxide (DTBP), a cetane improver. The unexpected finding of this work is that for many injection strategy calibrations, the more reactive fuel blends result in slightly lower exhaust temperatures. This effect is most pronounced at the 30% EGR level and best explained by the heat-release data shown in Figure I.1-4. Fuel reactivity has a clear impact on the combustion of the pilot mixture: more reactive fuels exhibit much higher rates of heat-release around top-dead center and more advanced heat-release associated with the main injection. However, the increase in exhaust temperature is attributed to late-cycle behavior after approximately 40 CAD ATDC. The least reactive baseline fuel results in the highest heat-release rates during this phase. This phenomenon appears to be associated with the relatively incomplete combustion of the pilot mixture; some of this mixture reacts very late in the cycle, such that less work is extracted from it. Thus, more energy is available as exhaust heat and the least reactive fuel results in the highest exhaust temperatures. Future studies will utilize full-boiling range fuels with a range of cetane ratings to provide a deeper understanding of how higher cetane enables better catalyst-heating performance.

Conclusions

The conclusions of this year's work are as follows:

- The baseline DSL piston can improve thermal efficiency and CFD simulations suggest that further improvements may be possible through changes in dimple design.
- Achieving high exhaust temperatures necessarily requires later, less efficient combustion phasing. Less reactive fuels may exhibit higher late-stage heat release rates due to incomplete combustion of the pilot injections early in the cycle.

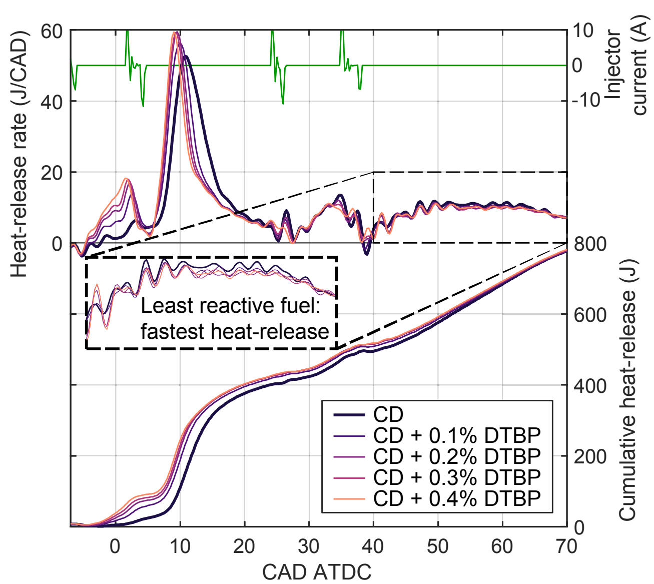


Figure I.1-4: Heat-release rate and cumulative heat-release as a function of crank angle degrees (CAD) after top dead-center (ATDC). The least reactive fuel shows the highest reaction rates during the later stages of combustion.

Key Publications

1. Perini, F., Busch, S., Reitz, R., and Wu, A., "Parallel Load Balancing Strategies for Mesh-Independent Spray Vaporization and Collision Models," *SAE Technical Paper* 2021-01-0412, 2021, https://doi.org/10.4271/2021-01-0412.

2. Busch, S., Wu, A. and Cho, S., "Catalyst-Heating Operation in a Medium-Duty Diesel Engine: Operating Strategy Calibration, Fuel Reactivity, and Fuel Oxygen Effects." SAE Technical Paper 2021-01-1182, 2021, DOI: https://doi.org/10.4271/2021-01-1182.

References

[1] 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, doi:10.4271/03-13-02-0016.

[2] 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.

[3] Busch, S. (2021) Medium-Duty Diesel Combustion. In U.S. DOE Advanced Engine and Fuel Technologies Program 2020 Annual Progress Report. pp. 31-37. Available online: https://www.energy.gov/eere/vehicles/articles/advanced-engine-and-fuel-technologies-fy-2020-annual-progress-report. Accessed 10/26/2021.

[4] Busch, S. (2020) Medium-Duty Diesel Combustion. In U.S. DOE Advanced Engine and Fuel Technologies Program 2019 Annual Progress Report. pp. 30-36. Available online: https://www.energy.gov/eere/vehicles/downloads/advanced-engine-and-fuel-technologies-fy2019-annual-progress-report. Accessed 10/27/2021

[5] Busch, S. (2019) Light- and Medium-Duty Diesel Combustion. In U.S. DOE Advanced Engine and Fuel Technologies Program 2018 Annual Progress Report. pp. 30-35. Available online: https://www.energy.gov/eere/vehicles/downloads/advanced-combustion-engines-and-fuels-fy2018-annual-progress-report-0. Accessed 10/27/2021.

Acknowledgements

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Acronyms, Abbreviations, Symbols, and Units

ATDC	After top-dead center
CAD	Crank angle degrees
CFD	Computational fluid dynamics
dCVC	Degree of constant-volume combustion
DSL	Dimpled stepped-lip
DTBP	Di-tert-butyl peroxide
EGR	Exhaust gas recirculation
SL	Stepped-lip
TDC	Top-dead center