

CFD-Guided Heavy Duty Mixing-Controlled Combustion System Optimization with a Gasoline-Like Fuel

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ABSTRACT

A computational fluid dynamics (CFD) guided combustion system optimization was conducted for a heavy-duty compression-ignition engine with a gasoline-like fuel that has an anti-knock index (AKI) of 58. The primary goal was to design an optimized combustion system utilizing the high volatility and low sooting tendency of the fuel for improved fuel efficiency with minimal hardware modifications to the engine. The CFD model predictions were first validated against experimental results generated using the stock engine hardware. A comprehensive design of experiments (DoE) study was performed at different operating conditions on a world-leading supercomputer, MIRA at Argonne National Laboratory, to accelerate the development of an optimized fuel-efficiency focused design while maintaining the engine-out NO_x and soot emissions levels of the baseline production engine. Compared to the base engine, the optimized results showed a significant improvement in closed-cycle, indicated specific fuel consumption (ISFC) across different engine speed and load points. When combined with modified injector configurations, the optimized piston bowl designs showed better in-cylinder air utilization and shorter combustion duration, thereby leading to improved fuel efficiency of up to 2.8%. In particular, increasing the injector hydraulic flow rate (larger nozzle diameter) was found to be beneficial by shortening the combustion duration while producing a higher incylinder combustion temperature for enhanced soot oxidation. A lower swirl ratio was also seen to be beneficial and the effects were attributed to the lower heat transfer loss and reduced need for fuel-air mixing. Increasing the compression ratio from 18.9 to 20.5 was also important for improving the fuel efficiency according to the relative contributions from key design parameters on ISFC.

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INTRODUCTION

Existing and future regulations focused on the reduction of greenhouse gas emissions are transforming both the transportation and refining industries. Engines and vehicles must become much more efficient and energy suppliers must adapt to changes in the market. Current projections indicate that the demand for gasoline products will decline due to the partial electrification of the passenger car fleet, while demand for diesel and middle distillate products will continue to rise as the global economy expands [1]. In order to lessen the impact of these long term trends and regulations, the efficiency of gasoline fueled engines must improve. One such efficiency improving technology is gasoline compression ignition (GCI) and much research is focused on the relationship between fuel properties and combustion under autoignition conditions. Fuels originating from the gasoline production stream with high volatility and low aromatic content have shown potential to reduce cradle-to-grave greenhouse gas emissions and criteria pollutants in compression ignition (CI) engines [2,3,4,5,6].

These gasoline-like fuels have a lower cetane number (CN) compared to diesel, which leads to longer ignition delay and better fuel-air mixing before the onset of combustion. Together with the lower aromatic content, lower soot can be obtained with these fuels. These longer ignition delays, however, can also lead to elevated pressure rise rates and peak cylinder pressures and the challenge becomes finding ways to harness the benefits while avoiding these penalties.

To date, the majority of published work has focused on the behavior of these fuels using production CI engines without significant modifications to engine hardware [7,8,9,10,11,12]. In this study, a computational fluid dynamics (CFD) guided combustion system optimization design was conducted for a model year 2013 Cummins ISX15 heavy-duty (HD) diesel engine and specifically tailored for a gasoline-like fuel that has an anti-knock index (AKI) of 58.

The fuel used is a straight-run naphtha which possesses gasoline-like physical properties. Previous experimental tests [5] have shown the advantages of this fuel on soot reduction while maintaining levels of efficiency and NO_x emissions comparable to ultra-low sulfur diesel (ULSD). The primary goal of the design exercise was to utilize the high volatility and low sooting tendency of the fuel to optimize the engine combustion system for improved fuel efficiency while maintaining engine-out NO_x within production levels. The CFD model was developed using the multi-dimensional CFD software package, CONVERGE, and the initial and boundary conditions were generated from a well-validated one-dimensional GT-Power model. Model predictions were validated against experimental results generated using the production engine hardware and showed very good agreement.

For the design optimization, the main variables included piston bowl geometry, compression ratio (CR), injector configuration and injection timing. Swirl ratio was also investigated as a secondary design variable. Design of experiments (DoE) and genetic algorithms (GA) are two popular and efficient optimization techniques in the engine industry. The GA method [13] is known to be efficient and effective when exploring optimum design strategies. However, the DoE method is capable of running more concurrent simulations and thus can achieve potentially shorter design times when sufficient computing resources are available [14]. In this study, a comprehensive DoE optimization was performed at different operating conditions on Argonne National Laboratory's supercomputer, MIRA, to accelerate the development of an optimized fuel-efficiency focused design. A systematic parametric study of the key design variables was also conducted to better understand the fuel effects on current heavy-duty mixing-controlled combustion systems.

ENGINE SPECIFICATIONS AND FUELS

A production MY2013 Cummins ISX 15 diesel engine was used as the base engine to understand the performance of the gasoline-like fuels under mixing-controlled combustion operation. General specifications for the engine are listed in Table 1, and more details are available in [5].

Table 1. Engine specifications

Displacement Volume	14.9 L
Number of Cylinders	6
Bore	137 mm
Stroke	169 mm
Compression Ratio	18.9 & 17.3
Diesel Fuel System	2500 bar common-rail
Air System	single-stage variable geometry turbocharger (VGT), high pressure cooled EGR, charge air cooler
Engine Ratings	336 kw (450 hp) @ 1800 rpm 2373 N-m (1750 lb-ft) @ 1000 rpm

Two fuels were considered in this study: a straight-run AKI58 naphtha and a market representative ULSD. The naphtha was chosen because it possesses physical characteristics similar to gasoline, but has a cetane

number relatively close to the minimum number available with market ULSD. This provides an opportunity to study fuels in the gasoline range without drastically altering the baseline engine's hardware configuration. Compared to ULSD, the naphtha fuel has higher volatility, lower viscosity, lower aromatic content, higher lower heating value (LHV) and a lower CN as shown in Table 2.

Table 2. Test fuels specifications

		Test Fuels	
		ULSD	Naphtha
IBP	°C	176	32
T10	°C	206	58
T50	°C	249	94
T90	°C	303	124
FBP	°C	337	140
Vapor Pressure	KPa	-	60.88
Density at 15.56 °C	g/mL	0.841	0.705
Kinematic viscosity	mm ² /s	2.25	0.58
Aromatics	vol%	29.7	9.1
Olefins	vol%	4.3	0.4
Saturates	vol%	66.0	90.5
Sulfur	ppm	11.9	19.3
H/C ratio	-	1.834	2.124
Cetane Number (CN)		43.7	33.7
RON	-	-	58.8
MON	-	-	57.9
AKI	-	-	58.4
Lower heating value	MJ/kg	42.818	43.363

DROP-IN TEST RESULTS

A previous study [5] has shown that using a straight run naphtha in this diesel engine led to appreciably lower soot compared to ULSD as shown in Figure 1(a), where a NO_x sweep is presented at the B50 operating point with a CR of 18.9. The data shows a lower filtered smoke number (FSN) for naphtha at different NO_x levels while maintaining diesel-equivalent brake thermal efficiency (BTE).

Utilizing the soot-NO_x trade-off, the lower soot of the naphtha fuel allowed the engine to be recalibrated from 3-4 g/hp-hr NO_x (production level) down to 1.5-2 g/hp-hr over the 12-mode non-idle Supplemental Emissions Test (SET) steady-state test cycle while maintaining "soot-free" (smoke ≤ 0.2 FSN) operation and reasonably good fuel efficiency as shown in Figure 1(b). A smoke number of 0.2 FSN (dashed black line in Figure 1(b)) roughly correlates to 0.01 g/hphr, the US EPA particulate matter (PM) tailpipe emission standard for on-highway heavy-duty engines. The speed and load ranges for the 12 modes are roughly from 1135 - 1600 rpm and 5 - 20 brake mean effective pressure (BMEP).

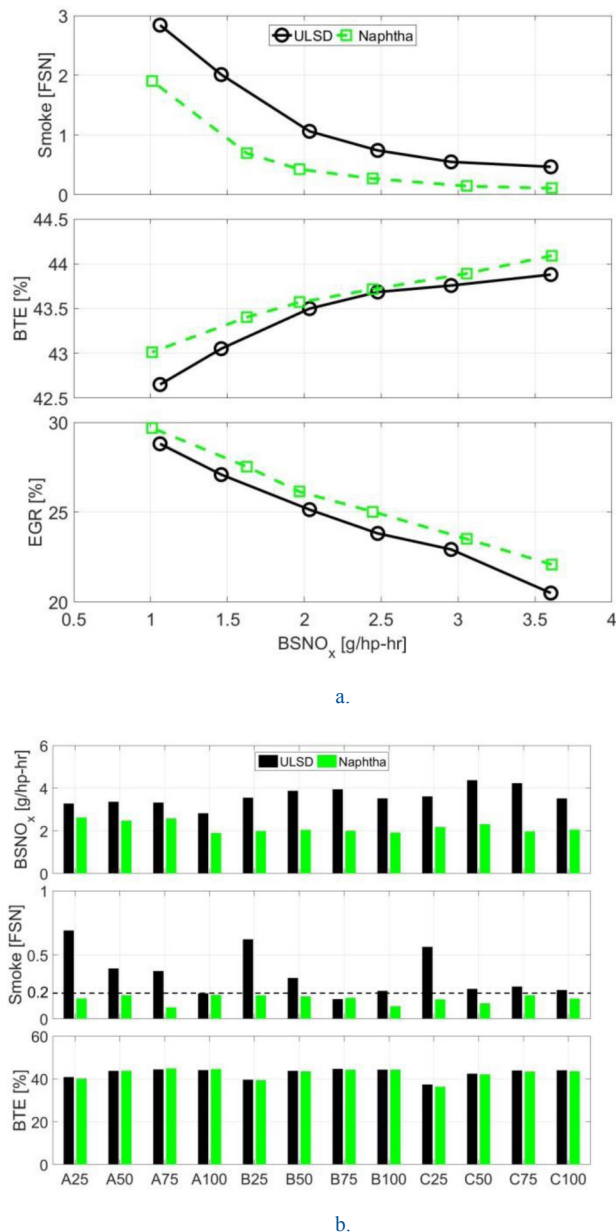


Figure 1. Drop-in test results of ULSD and naphtha (a) at B50 and (b) over the 12-mode non-idle SET steady-state test cycle at CR 18.9 [5]

CFD modeling was used to take a closer look at the B50 naphtha operating point in an effort to better understand the improvement in soot emissions. The formulation of the CFD model will be described in the following section. Figure 2(a) plots the percentage of different bands of equivalence ratio (Φ) in mass fraction at different crank angles (CA) for the two fuels tested and essentially indicates how well the air in the combustion chamber is utilized. The chart shows the better air utilization of naphtha through reduced rich regions ($\Phi > 1.5$) and elevated lean regions ($0.5 < \Phi < 1$), especially during the phase where intense combustion happens. This is likely due to the naphtha's gasoline-like fuel properties, i.e., high volatility and low viscosity. As a consequence, significantly lower soot was generated in the combustion chamber as shown in Figure 2(b). These experimental

and simulated findings [5,6] suggested that additional improvements in efficiency and emissions could be realized through a design optimized for the fuel's properties.

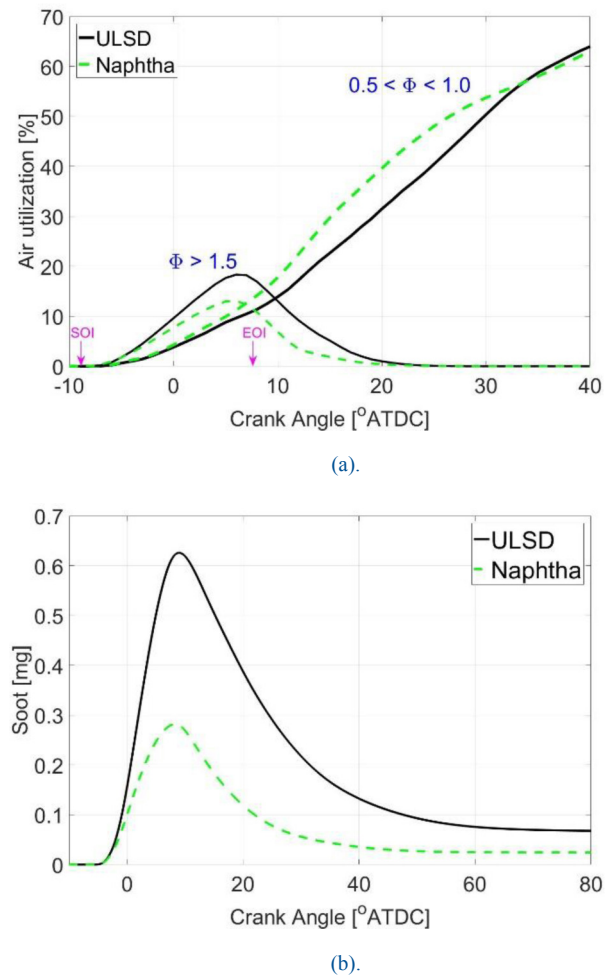


Figure 2. Comparison of (a) air utilization and (b) soot evolution for ULSD and naphtha at 2 g/hp-hr NO_x B50 condition

COMBUSTION SYSTEM DEVELOPMENT METHODOLOGY

The analysis-led design process involves a close coupling between the 3-D CFD in-cylinder combustion development and the 1-D engine cycle analysis. The focus of this study is to conduct a 3-D CFD-guided combustion system hardware development to generate the initial designs of the piston bowl geometry and the injector spray pattern. Engine hardware will then be fabricated according to these designs and evaluated experimentally. Subsequently, the CFD-guided designs will be further refined based on the engine test results. The current study is the first step in this iterative optimization process.

The following is an overview of the CFD-guided design process undertaken in the study:

- Model formulation and validation:
 - Set up the CFD model
 - Calibrate spray and emissions models against experimental data

- Bowl concepts generation
 - Generate bowl concepts while maintaining compression ratio and squish height
- Pre-DoE parametric study
 - Initial concepts evaluation
 - Identify key design parameters
 - Define proper DoE design space for key design parameters
 - Define emissions targets and engine mechanical limits
- DoE optimization
 - Select proper sampling methods, then generate and run DoE cases
 - Construct response surface model (RSM)
 - Identify optimal cases from RSM and perform validation in CFD
 - Conduct sensitivity analysis for key design parameters

The details of each step will be described in the following sections.

Model Formulation

The model formulation has been discussed in the previous study [6] and will be briefly reviewed here. A list of the models used and some details are shown in Table 3. Briefly, the commercial CFD software, CONVERGE version 2.3.8, was used to formulate the model. It features automatic mesh generation, detailed combustion models, high-fidelity spray models and a wide variety of emissions models, and offers rapid turnaround time for model building when designing the bowl geometry or changing the angle of sector mesh [15].

A Reynolds averaged Navier-Stokes (RANS)-based re-normalization group (RNG) k - ϵ turbulence model was used in conjunction with a detailed chemistry combustion model [16]. Although large eddy simulation (LES) could potentially deal with large disparities of length scales and complicated geometries, and may be more accurate than RANS [17], the choice of a RANS-based method is mainly due to the computational resources required to run the large number of DoE simulations for the optimization work.

A traditional Lagrangian spray model was used assuming a “Blob” injection method. It is very computationally efficient because it injects liquid parcels (a group of droplets with identical properties) to statistically represent the spray field in the combustion chamber using a specific rate of injection (ROI) profile. However, this traditional method cannot capture the dynamics upstream of the nozzle exit, i.e., the needle motion (or “wobble” effect), which is known to lead to injector hole-to-hole variation [18]. Coupling the in-nozzle flow effect (e.g., “one-way coupling” method [19]) in design work is an interesting area to explore. Both the Kelvin-Helmholtz (KH) [20] and Rayleigh-Taylor (RT) [21] algorithms were adopted for secondary break-up process while the no-time counter (NTC) model [22] was used for collision process. The Frossling correlation was used to account for the droplet evaporation [23] and the fuel liquid properties were generated from Aspen HYSYS [24].

Although it treats the turbulence-chemistry-interaction (TCI) as a simple delta function, the detailed combustion model is superior in its simplicity and robustness in calculation, and is suitable for many

simulations with complicated geometry and multi-physics (e.g., multicomponent fuel and multi-phase flow). Moreover, the importance of TCI in engines is still to be evaluated systematically although many studies have suggested the importance in constant-volume chamber spray flames under diesel-engine relevant conditions [25,26,27,28,29]. Poor prediction of ignition in less reactive conditions is one possible limitation of the detailed combustion model. However, this might not be a concern in the current study as the environment in the cylinder when fuel is injected is very reactive (e.g., ~ 1000 K temperature and 72 bar pressure at B50). The chemical mechanism for naphtha used a primary reference fuel (PRF) mechanism from Liu et al. [30] and the one for ULSD was from an n-heptane surrogate mechanism [31]. Although there are other detailed models available, the choice of these two mechanisms is mainly because they are highly computationally efficient and widely adopted in the industry.

Regarding the emissions models, an empirical Hiroyasu-NSC (Nagle and Strickland-Constable) model was used for the soot formation and oxidation prediction with C_2H_2 as the soot precursor [15,32]. There are more detailed soot models available for engine simulations such as the particulate mimic (PM) model [33] based on moment method and particulate size mimic (PSM) model [34] based on sectional method. However, the increased computational requirement makes the use of detailed soot models in a large optimization study infeasible at the current stage. The NO_x prediction used a 4 species and 13 reaction reduced mechanism [35].

Table 3. Computational models setup

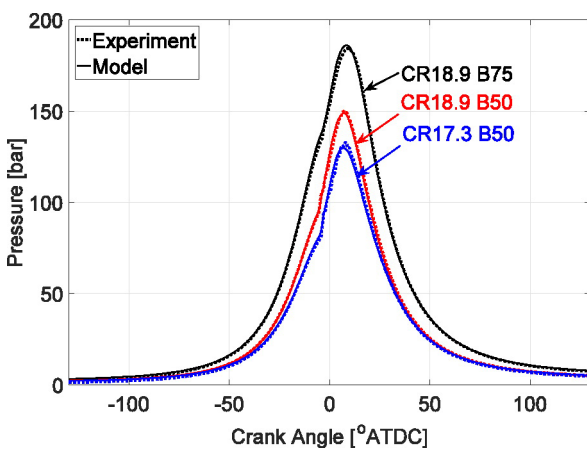
CONVERGE 2.3.8	
Dimensionality	3D with Adaptive Mesh Refinement
Grid Details	Base grid: 1.0 mm Smallest grid size: 0.25 mm Gradient-based AMR on velocity and temperature Fixed embedding near nozzle region: 0.25 mm
Total Cell Count	Sector: 300,000 Full: 2.8 million
Turbulence	RNG k - ϵ RANS
Wall Heat Transfer	O'Rourke & Amsden
Spray Models	Injection: Blob Break-up: KH-RT Collision: NTC Evaporation: Frossling correlation Liquid properties generated from HYSYS
Time Step	Variable time step
Combustion Model	Detailed chemistry combustion model
Chemical Mechanism	Naphtha (AKI58): Liu et al. PRF mechanism with 44 species and 139 reactions ULSD: Chalmers n-heptane mechanism with 42 species and 283 reactions
Emission Models	Soot: Hiroyasu-NSC NO_x : Detailed chemistry NO_x model

A gradient-based adaptive mesh refinement (AMR) was used based on velocity and temperature fields to refine the regions necessary, while leaving the cells in the less important regions relatively coarse. This significantly reduced the computational cost while maintaining the high fidelity of the simulations. A fixed-embedding strategy was used to resolve the regions close to the nozzle exit. Sector meshes were used for the massive DoE runs and 360 degree meshes were used where necessary, for example, to accurately capture the effect of

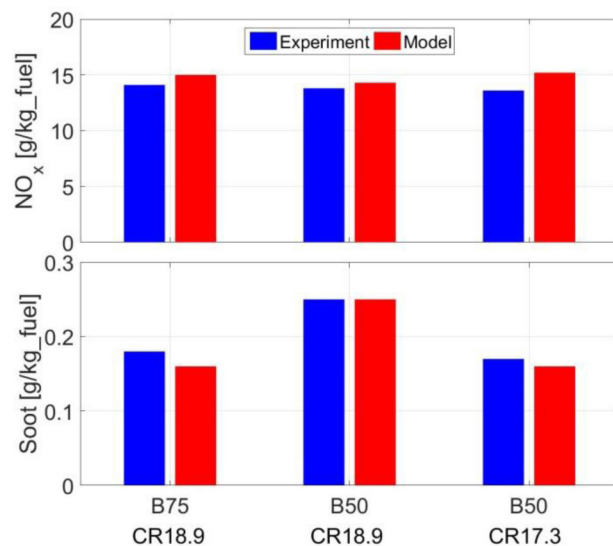
the number of nozzle holes and swirl ratio in the validation process. The boundary conditions were generated from a well-validated 1-D GT-Power model.

Model Validation

The formulated CFD model was validated against experiments at different loads and compression ratios for both fuels. The validation for ULSD has been shown in a previous study [6] and will not be presented here. Figure 3(a) and (b) plot the comparison of experimental and simulated results for the cylinder pressure trace and emissions, respectively, at different operating conditions and compression ratios for naphtha. It can be seen that the predictions are in fairly good agreement with the experimental data and provide confidence that the comprehensive design optimization will be valid.



(a).



(b).

Figure 3. Comparison of experimental results and numerical predictions for (a) cylinder pressure trace and (b) emissions at different operating loads and different compression ratios for naphtha

Design Space and Constraints

The design space and constraints were identified in the pre-DoE process. More than 20 designs were initially evaluated and 6 were down-selected for the DoE design optimization. This step requires the identification of design space for key design parameters for each bowl geometry at different operating conditions. It is a tedious and labor intensive step in the process.

Four operating conditions were considered in this study, including B50, B75, A75 and C100, covering frequently used conditions for a long-haul truck. The following is a summary of the design parameters and their design space:

- Bowl geometry and compression ratio (18.9 - 20.5) with 6 bowl geometries down-selected from more than 20 designs were studied
- Number of nozzles (8 - 9 - 10) for the injector
- Total nozzle area (TNA) (1 - 1.15 - 1.3) assuming the stock injector TNA is 1 and scaling it up to 1.3. The rate of injection (ROI) profile was also changed when TNA was varied.
- Nozzle inclusion angle variation depending on bowl geometry
- Start of injection (SOI) variation depending on bowl geometry and operating condition
- Swirl ratio (secondary) was not included in the design space, but studied as a variable after the DoE process and was found very promising in improving fuel efficiency

The design strategy was to conduct optimization for each bowl at each operating condition aiming for the lowest ISFC with the constraints of:

- Maximum pressure rise rate (MPRR) < 10 bar
- Peak cylinder pressure (PCP) < 220 bar
- Soot < 0.045 g/hp-hr
- NOx < 3 g/hp-hr

DoE Optimization on MIRA Supercomputer

A stratified Latin hypercube sampling method was used to sample the design space. With this even sampling method, one has better control over the distribution of design space while managing the computational cost. An example of the sampling is shown in Figure 4. Around 80 samples for each operating condition with each bowl design were generated and fed into a script to generate the CFD input files. In total, more than 2000 simulations were performed for the optimization design. To accelerate the development process, one of the fastest supercomputers in the world, Argonne National Laboratory's MIRA, was utilized to conduct this computationally intensive design optimization. Previously, Kodavasal et al. [36] had used this supercomputer to perform a global sensitivity analysis for a gasoline compression ignition system in order to understand the uncertainties arising from different sources.

MIRA is an IBM Blue Gene/Q supercomputer with a total number of 786,432 cores. It has 48 racks with each rack containing 1024 computing nodes and each node using a 1600 MHz processor with 16 cores. In this study, each sector simulation used 32 cores and 256