

Computational Optimization of Reactivity Controlled Compression Ignition in a Heavy-Duty Engine with Ultra Low Compression Ratio

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ABSTRACT

Many studies have demonstrated ability of low temperature combustion to yield low NO_x and soot while maintaining diesel-like thermal efficiencies. Methods of achieving low temperature combustion are numerous and range from using high cetane number fuels, like diesel, with large amounts of exhaust gas recirculation, to completely premixing a high octane number fuel, like gasoline, and approaching an HCCI-like condition. Both of the aforementioned techniques have relatively short combustion duration that results in very a rapid rate of heat release, and hence very rapid rates of pressure rise. This has been one of the major challenges for premixed, low temperature combustion at mid and high load. Reactivity Controlled Compression Ignition (RCCI) has been introduced recently, which is a dual fuel partially premixed combustion concept. In this strategy in-cylinder fuel blending is used to develop fuel reactivity gradients in the combustion chamber that result in a broad combustion event and reduced pressure rise rates. RCCI has been demonstrated to yield low NO_x and soot with high thermal efficiency in a heavy-duty engine using a compression ratio of 16.1 at loads up to 15 bar gross IMEP. However, extension to full-load operation has proven to be difficult with a high compression ratio. The objective of this work was to optimize the engine with a low compression ratio of 11.7 using computational tools. The KIVA3V-CHEMKIN code, a multi-dimensional engine CFD model was coupled to a Nondominated Sorting Genetic Algorithm (NSGA II), which is a multi-objective genetic algorithm. Three engine operating conditions were investigated in this study, a low-load, mid-load, and a high-load point, 4, 9, and 23 bar gross IMEP, respectively. The goal of the optimization study was to simultaneously reduce six objectives, which are soot, NO_x, unburned hydrocarbons,

carbon monoxide, indicated specific fuel consumption, and the maximum pressure rise rate. The genetic algorithm was allowed to vary six engine design parameters, namely percent premixed gasoline, EGR fraction, and diesel direct injection parameters.

INTRODUCTION

The direct injection compression ignition (DICI) engine has a superb reputation for its fuel economy, reliability, and durability. However, due to the heterogeneous nature of conventional diesel combustion, particulate matter (soot) and nitric oxide (NO_x) emissions have been a challenge for diesel engines. In addition, improving fuel efficiency is always a goal because of its direct connection to CO₂ emissions and crude oil usage. Hence, the heavy-duty diesel engine has been a topic of massive research and development over the last two decades. The emissions consequences of conventional DICI mixing limited combustion can be best illustrated on a local Φ - local Temperature space diagram, which is shown in [Figure 1](#) [1]. The “Conventional diesel” line in [Figure 1](#) represents a snapshot in time of a burning diesel spray in a 21% O₂ environment. It can be seen that there is a diffusion flame (i.e., mixing controlled burning) at stoichiometric mixture, which yields high NO_x formation rates, and a region of $2 < \Phi < 3$ with $T \sim 1800$ K, which can produce unacceptably high soot formation rates.

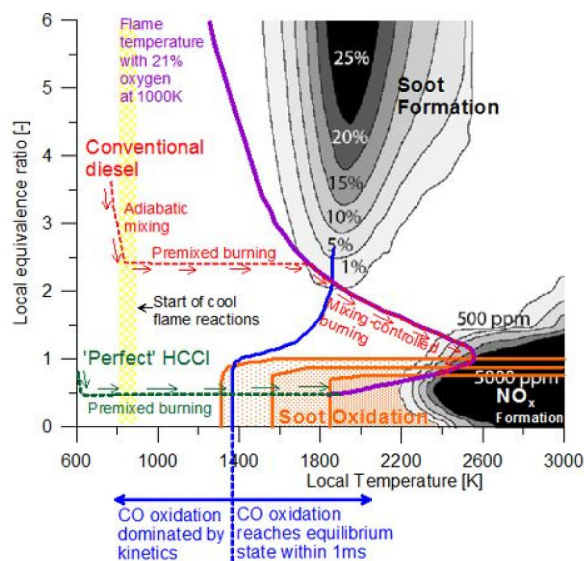


Figure 1. Local Equivalence Ratio vs. Local Temperature for Conventional Diesel Combustion [1].

In an effort to reduce NO_x and soot emissions, while maintaining high thermal efficiency, many new compression ignition combustion strategies have been proposed. Homogeneous Charge Compression Ignition (HCCI) is a concept that has been researched for over 20 years and was initially studied in four-stroke engines by Foster et al. in 1983 [2]. HCCI combustion has been shown to have superior characteristics in terms of thermal efficiency, which results from lower heat transfer losses and shorter combustion durations [3]. In addition, the lean, low temperature combustion process yields near zero NO_x and soot emissions, which are depicted in Figure 1 as 'perfect' HCCI. Although HCCI combustion appears thermodynamically attractive, the HCCI concept presents a controllability challenge, as it gives up two combustion control aspects. First, the timing of ignition is not controlled, either by fuel injection, as in a DIC engine, or by the spark, as in a SI engine. Second, the rate of heat release is not controlled, either by the rate of fuel injection, as in a DIC engine, or by finite turbulent flame propagation, as in a SI engine. As a result, the near constant volume combustion event can lead to a very rapid rate of heat release, and hence a very rapid rate of pressure rise. These advantages and challenges of HCCI combustion have motivated the investigation of Partially Premixed Compression Ignition (PPCI).

As indicated in Figure 1, to avoid the high NO_x and soot formation rates, the fuel must have sufficient time to mix before ignition takes place. In the case of PPCI the fuel is injected either very early or late in the cycle to promote mixing before ignition. Diesel PPCI was characterized by researchers at Lund University at 8, 12, and 15 bar gross

indicated mean effective pressure¹ (IMEP) [4]. They found that the traditional NO_x-soot trade-off that exists with conventional DIC diesel combustion can be defeated with diesel PPCI, but at the cost of a decline in combustion efficiency. By using EGR rates in excess of 60%, the NO_x emissions are near zero and the soot emissions began to decline sharply. Unfortunately, these high EGR levels resulted in combustion efficiencies below 90%.

Another approach is to use low reactivity fuels to allow for more mixing time before ignition. Kalghatgi was one of the first [5] to operate a heavy-duty compression ignition engine with conventional gasoline. More recently, researchers at Lund University have been studying gasoline PPCI in a heavy-duty engine from low to high load. Manente et al. [6, 7] have developed an operating strategy very similar to UNIBUS [8] to operate a heavy-duty DIC engine with gasoline. Their strategy utilizes two direct injections, high boost, and approximately 50% EGR. At 18 bar gross IMEP they were able to achieve soot in range of 1-2 FSN, gross indicated efficiency of 56%, NO_x below 0.3 g/kW-hr, and maximum pressure rise rates (MPRR) around 15 bar/deg. These results are promising as they were achieved essentially across the entire load range.

Additionally, Dempsey and Reitz [9] have conducted a genetic algorithm optimization of gasoline PPCI operation in a heavy-duty compression ignition engine at mid and high-load with the stock compression ratio of 16.1. It was shown that the mid-load condition exhibits low emissions, gross indicated thermal efficiency of 50%, and acceptable maximum pressure rise rate. At the high-load condition, while achieving low NO_x emissions and an efficiency of 50% as well, soot and maximum pressure rise rate remain challenging for gasoline PPCI combustion. This is consistent with the findings of the experimental studies conducted at Lund University that were mentioned previously.

The aforementioned studies have shown that PPCI, using gasoline or diesel fuel, can yield low emissions, excellent fuel efficiency, and acceptable maximum pressure rise rate from low to mid-load. However, due to the large amounts of EGR required with diesel fuel, extension to high load is not practical. With gasoline, it has been shown that high-load operation is achievable, but a strong trade-off exists between maximum pressure rise rate and soot emissions [9].

Bessonette et al. [10] demonstrated experimentally that the best fuel for HCCI operation has autoignition qualities between that of diesel fuel and gasoline, depending on the operating condition. For instance, they demonstrated that at 16 bar BMEP² the most suitable fuel was in the gasoline boiling range and had a derived cetane number of ~27 (i.e.

¹Gross refers to the compression & expansion strokes only (-180° ATDC to 180° ATDC). Indicated means the cycle work was calculated from the cylinder pressure, neglecting engine friction. Mean Effective Pressure is equal to the cycle work divided by the engine displacement volume.

octane number of 80.7). However, at 2 bar BMEP a cetane number of ~ 45 (i.e., a traditional diesel fuel) was required for stable operation. Thus, it seems that exploring fuel blends for specific operating conditions would be beneficial. Inagaki et al. [11] were one of the first to successfully demonstrate dual fuel PPCI using in-cylinder fuel blending. They discovered that the ignition timing could be controlled by changing the ratio of the two fuels and that with injection timings of about 30° before top dead center (BTDC) combustion rates were mild compared to HCCI using a single fuel. Later injections led to unacceptably high NO_x emissions, while earlier injections led to very high pressure rise rates. However, using a compression ratio of 14, they were able to operate the engine up to 12 bar IMEP using iso-octane and diesel fuel with no EGR, yielding 10 ppm of NO_x and a 0.1 FSN, which is low soot.

Learning from the dual fuel research of Bessonette et al. and Inagaki et al., Kokjohn, Hanson, Splitter, and Reitz [12,13,14,15] successfully demonstrated clean and extremely efficient dual fuel combustion in a heavy-duty Caterpillar single-cylinder engine. Guided by computational tools, they discovered that the high pressure rise rates seen by Inagaki et al. [11] could be avoided by using optimized multiple injections with even earlier injection timings than they had used [16]. This allowed them to develop a gasoline/diesel in-cylinder fuel blending strategy that provided low emissions (below EPA 2010 levels, in-cylinder) and a peak net cycle efficiency of 53% from 4 bar to 14.5 bar IMEP. This combustion strategy was called Reactivity Controlled Compression Ignition (RCCI) based on the findings of Kokjohn et al. [17], where it was discovered that in-cylinder fuel blending reduces the maximum pressure rise rate compared to single fuel premixed combustion due to optimized reactivity gradients established in the chamber. However, extension to loads beyond 14.5 bar IMEP has proven difficult because of maximum pressure rise rate constraints and increased EGR rate requirements. Hence the main focus of the present work was to explore RCCI combustion in a heavy-duty engine up to full load (~ 23 bar IMEP) using a reduced compression ratio piston with CR = 11.7, without sacrificing the good fuel efficiency and low emissions seen at lower loads.

COMPUTATIONAL TOOLS

MULTI-DIMENSIONAL ENGINE CFD

In this work the KIVA-CHEMKIN code, which is based on the KIVA3V Release 2 code, was used [18,19,20]. The KIVA3V code uses the Lagrangian-Drop Eulerian-Fluid approach for modeling engine sprays, in which liquid fuel is treated as a Lagrangian parcel and the ambient gas is

discretized into cells. The physical properties of gasoline and diesel fuel (for spray break-up, evaporation, and mixing) are taken to be those of iso-octane ($i\text{-C}_8\text{H}_{18}$) and tetradecane ($\text{C}_{14}\text{H}_{30}$), respectively. Several sub-model improvements have been made to the KIVA3V code, including fuel droplet break-up, droplet evaporation, droplet collision modeling, turbulence modeling, grid independent spray models, and the development of primary reference fuel chemical mechanisms, as summarized next.

Beale and Reitz [21] implemented a hybrid spray break-up model, namely the KH-RT model. The droplet collision model is from the original KIVA3V code and is based on O'Rourke's model. However, a radius-of-influence method was implemented to reduce the mesh dependency of the collision process [22]. The interaction of the liquid fuel parcels with the wall was modeled with the standard KIVA3V wall film model developed by O'Rourke and Amsden [23]. Ra and Reitz [24] made improvements to the droplet vaporization sub model. The RNG $k\text{-}\epsilon$ turbulence model was modified and implemented into the KIVA3V code by Han and Reitz [25]. In order to reduce the grid size dependence of the Lagrangian spray model, the GASJET model of Abani et al. [22] was used to model the relative velocity between the fuel droplets and the gas phase. Finally, to further reduce the simulation time, a dynamic maximum timestep strategy was implemented [9].

The KIVA-CHEMKIN code has been coupled to the CHEMKIN II libraries for detailed combustion chemistry calculations [26]. Conventional gasoline and diesel fuels are multi-component fuels and consist of a wide range of hydrocarbon species, and it is thus not practical in engineering applications to kinetically model each species in the real fuel. Therefore, the ignition and combustion characteristics of automotive fuels are typically represented by blends of the primary reference fuels (PRF), namely iso-octane and n-heptane ($n\text{-C}_7\text{H}_{16}$). In this work, the ignition and combustion characteristics of iso-octane and n-heptane are used to model the kinetics of gasoline and diesel fuel, respectively. Using single component fuel surrogates to represent the fuel chemistry of gasoline and diesel fuel is certainly a modeling simplification, but, as will be shown in a later section, this modeling approach does accurately capture the combustion characteristics of dual-fuel RCCI combustion. A reduced PRF mechanism consisting of 45 species and a 142 reactions, which includes NO_x chemistry, was utilized in this study to represent the autoignition and subsequent combustion of gasoline and diesel fuel [27]. Soot emissions were predicted using a phenomenological soot model. Two competing processes are considered in the model, namely soot formation and soot oxidation. Acetylene (C_2H_2) is used

² Brake Mean Effective Pressure is equal to the cycle work divided by the engine displacement volume, where the cycle work is obtained from a dynamometer, and thus includes engine friction.

as the soot inception species in the formation rate equation [28]. The NO_x formation chemistry is represented by 4 species and 12 reactions, which is a reduced version of the GRI NO_x mechanism [29].

OPTIMIZATION METHODOLOGY

In this work the optimization tool used was based on genetic algorithms (GA). Genetic algorithms are mathematical algorithms that are designed to simulate the evolutionary process of an ecosystem, which obeys the Darwinian idea of “survival of the fittest”. It is a search-based algorithm that utilizes the “fittest” attributes of previously simulated designs to generate new designs. The goal is to create designs that move the evolutionary process towards better solutions. In an attempt to mimic natural evolution and to avoid localized optimization, random changes of genes are introduced as well. Therefore, GAs are considered global optimization techniques because they explore the entire design space.

Shi and Reitz [30] assessed the performance of three different Multi-Objective Genetic Algorithms (MOGA) used in DICI diesel engine optimization. Considering that the goal of the optimization is to find a set of designs that are as close as possible to the true Pareto front and have solutions that are diverse as possible, they defined four quantities for assessing MOGAs. Their analysis concluded that the Nondominated Sorting Genetic Algorithm II (NSGA II) of Deb et al. [31] with a large population size displayed better performance in approaching the true Pareto front and spreading the optimal solutions over all the objectives. In addition, the genetic operators (crossover and mutation) and their respective settings remain unchanged from the previous study [30].

When studying multi-objective problems trade-offs exist from design to design. For example, an engine design that yields low fuel consumption and low acoustic noise might have high emissions. This raises the question: what is an optimal solution in a multi-objective problem? The most common definition for “optimum” used in these types of problems is referred to as Pareto optimal. In words, a solution set (i.e., all the objectives) is Pareto optimal if there exists no other solution set which would decrease one of the objectives without causing a simultaneous increase in any other objective. This idea is illustrated for an optimization with only two objectives in Figure 2 [30].

In Figure 2 A-H are solutions to a two objective optimization problem. It can be seen that solutions A-D are Pareto optimal because they provide a simultaneous decrease in both the objectives, as compared to solutions E-H. This “front” of optimum solutions is typically referred to as the Pareto front. In addition to understanding what an optimum solution is, quantifying when the optimization has converged on a set of Pareto optimal solutions is necessary. The convergence of the GA was monitored in this work as was done in an earlier

optimization by Kokjohn and Reitz [32]. Essentially, when the Pareto front (A-D) stops advancing towards the origin of Figure 2, the optimization is said to have converged. The convergence parameter that quantifies the movement of the Pareto front is presented later.

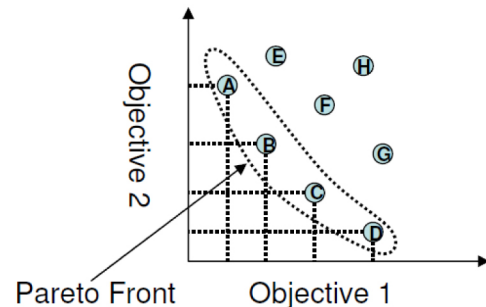


Figure 2. Concept of Pareto Optimal Solutions for a Two Objective Optimization.

Considering that GA optimizations are searched based and the goal is to find diverse solutions, typically there are a large number of evaluations that are not on the Pareto front. However, these evaluations are not necessarily wasted because they contain valuable information about the effects that design parameters have on the objectives across the entire design space. Unfortunately, it can be difficult to visualize this information in problems that contain more than two objectives, as in this study. Therefore a non-parametric regression technique was utilized to post-process the optimization results. A non-parametric regression tool is simply a curve fitting technique that can be applied to an irregular set of data where the functional form is unknown. The tool used in this study is known as the Component Selection and Smoothing Operator (COSSO), which was developed by Lin and Zhang [33] and successfully demonstrated on CFD engine simulation results by Liu and Reitz [34].

ENGINE CFD MODEL VALIDATION

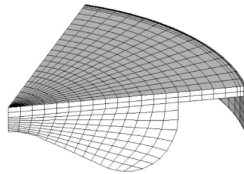
Before conducting the genetic algorithm optimization, the KIVA3V-CHEMKIN code was validated against experimental data of gasoline/diesel RCCI combustion in a heavy-duty compression ignition engine that utilized the stock compression ratio (CR) of 16.1. The engine geometry and diesel injector specifications are given in Table 1 and the computational grid's specifications are in Table 2.

Table 1. Caterpillar Engine & Injector Specifications
[14].

Engine Geometry	
Displacement [L]	2.44
Bore x Stroke [mm]	137.2 x 165.2
Connecting Rod [mm]	261.6
Compression Ratio	16.1
Swirl Ratio [-]	0.7
Diesel Fuel Injector	
Number of Holes	6
Hole Diameter [micron]	250
Included Spray Angle [deg]	145

Table 2. Computational grid at top dead center for stock engine configuration (60 degree sector mesh).

Computational Grid	
Cells at IVC	8300
Average Cell Size	~ 3 mm
Azimuthal Resolution	4 degrees
Approximate Run Time	~ 15 hrs.



As mentioned earlier, extensive RCCI experimental and computational research has been conducted at a variety of operating conditions using the stock Caterpillar engine described in Table 1. Three of these operating conditions were chosen to aid in validating the computational model: namely 5.2 bar IMEP [13], 9 bar IMEP [14], and 14.5 bar IMEP [15], the details of which are outlined in Table 3.

A comparison of the KIVA-CHEMKIN predicted cylinder pressure and apparent heat release rate (AHRR) to the experiments for the RCCI load sweep is shown in Figure 3. In addition, the emissions results across the load sweep are also shown in Figure 4. As can be seen from the plots, the KIVA-CHEMKIN model does an excellent job at capturing the combustion characteristics and resulting emissions of RCCI from low-load to 14.5 bar IMEP. The only point of concern is the soot prediction at 14.5 bar IMEP. As indicated in Table 3, this operating condition is very near stoichiometric combustion (global equivalence ratio of 0.97). This suggests that perhaps different soot modeling constants or soot inception species should be used for lean and rich combustion. However, since the primary focus of this work is RCCI combustion development, this was not explored. It is noted however that the soot emissions might be over predicted as stoichiometric operation is approached.

Table 3. Engine operating conditions for a gasoline/diesel RCCI load sweep from 5.2 to 14.5 bar gross IMEP using compression ratio of 16.1.

Operating Conditions	5.2 bar IMEP	9 bar IMEP	14.5 bar IMEP
Speed [rpm]	1300	1300	1300
Premixed Gasoline (Mass %)	68%	89%	90%
DI Diesel Injection #1 [ATDC]	-58	-58	-58
DI Diesel Injection #2 [ATDC]	-37	-37	-37
Percent Diesel in Inj. #1 [%]	62%	64%	37%
EGR Rate (%)	0%	43%	57%
Intake Temperature [C]	32	32	32
Intake Pressure [bar abs.]	1.38	1.75	2.34
IVC/EVO [ATDC]	-143/130	-143/130	-85/130
Exhaust Pressure [bar abs.]	1.45	1.84	2.52
Air Fuel Ratio [-]	60.0	29.0	15.1

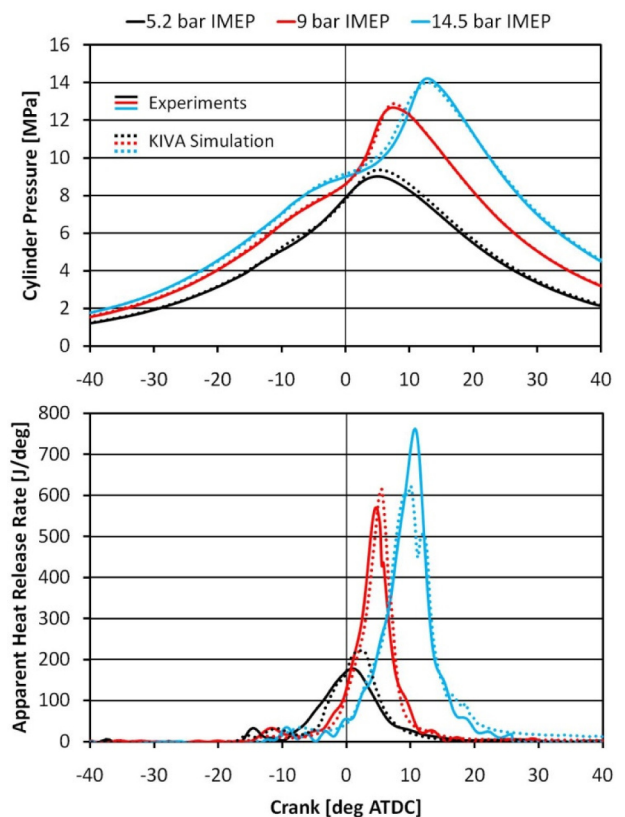


Figure 3. Experiments and simulation of gasoline/diesel RCCI over a load sweep conducted in the stock Caterpillar engine.

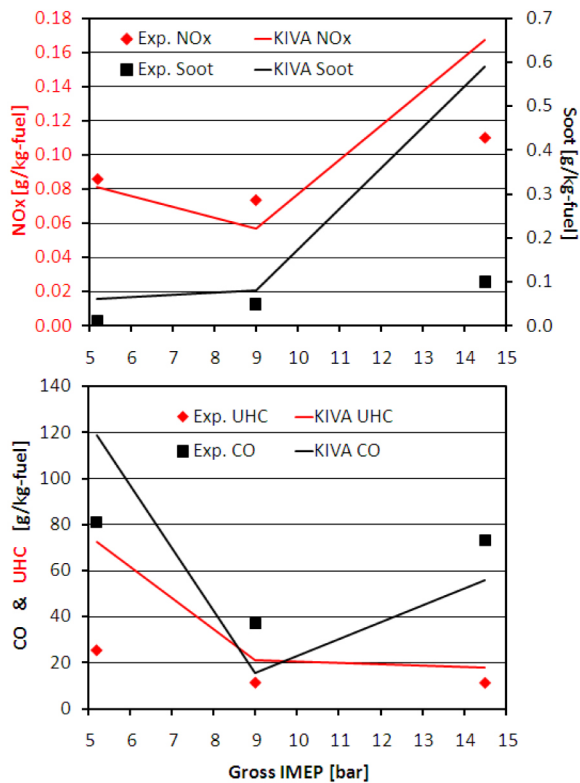
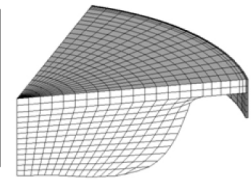


Figure 4. Experimental and simulated emission results of gasoline/diesel RCCI over a load sweep conducted in the stock Caterpillar engine.

Table 4. Computational grid at top dead center for the reduced compression ratio piston (60 degree sector mesh).

Computational Grid	
Cells at IVC	9700
Average Cell Size	~ 3 mm
Azimuthal Resolution	4 degrees
Approximate Run Time	~ 15 hrs.



Three engine operating conditions were optimized in this study, a low-load, mid-load, and a high-load point, which are approximately 4, 9, and 23 bar gross IMEP, respectively. The conditions that were fixed throughout the optimization are shown in Table 5. The genetic algorithm was allowed to vary the six engine design parameters, shown in Table 6.

Table 5. Fixed engine operating conditions during optimization.

Operating Conditions	Low-Load	Mid-Load	High-Load
Speed [rpm]	800	1300	1800
Fuel [mg/cycle]	48	94	270
Gross IMEP [bar]	~ 4	~ 9	~ 23
Intake Temp. [C]	60	60	60
Intake Press. [bar abs.]	1.0	1.75	3.0

Table 6. Engine design parameters & ranges for three load RCCI optimization.

Design Parameter	Low-Load	Mid-Load	High-Load
Premixed Gasoline [%]	10 to 95	30 to 95	60 to 95
DI Diesel SOI #1 [ATDC]	-100 to -50	-100 to -50	-100 to -30
DI Diesel SOI #2 [ATDC]	-40 to 0	-40 to 0	-15 to 10
Diesel Fuel in 1st Inj. [%]	0 to 100	0 to 100	0 to 100
Diesel Inj. Press. [bar]	300 to 1500	300 to 1500	300 to 1500
EGR [%]	0 to 60	0 to 60	0 to 50

In this study the EGR gases were assumed to be complete combustion products of hydrocarbon fuels in air, namely O_2 , N_2 , CO_2 , and H_2O . The relative amounts of each were determined in an iterative process assuming the combustion of a mixture of iso-octane (i.e., gasoline), tetradecane (i.e., diesel fuel), air, and EGR gases at the conditions specified in Table 5. The resulting initial gas composition is shown in Figure 6 as a function of the EGR rate specified by the GA. The H_2O and CO_2 concentrations were nearly identical, so only the CO_2 amount is shown in the plot. It can be seen that, because the boost pressure is fixed (based on reasonably expected turbocharger efficiencies), the global equivalence ratio varies.

GENETIC ALGORITHM OPTIMIZATION

The genetic algorithm optimization was conducted on the same Caterpillar engine as discussed previously, except with a constant intake valve closure (IVC) time of -143° ATDC, and a reduced compression ratio of 11.7. In order to accomplish the low compression ratio, the squish height was reduced and the central pip of the piston bowl was essentially removed [35]. Figure 5 compares the stock piston (CR = 16.1) to the newly designed piston (CR = 11.7) at top dead center. In addition, the computational grid and its properties for the reduced compression ratio are shown in Table 4.

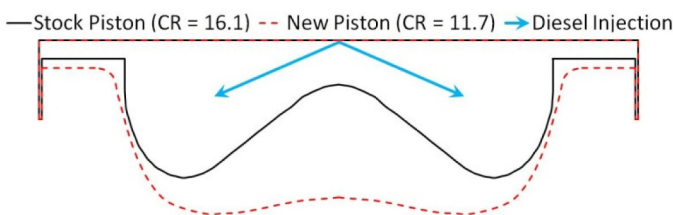


Figure 5. The Caterpillar stock piston bowl shape (CR = 16.1) vs. the reduced compression ratio design explored in this optimization study (CR = 11.7).