

Heavy-Duty RCCI Operation Using Natural Gas and Diesel

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ABSTRACT

Many recent studies have shown that the Reactivity Controlled Compression Ignition (RCCI) combustion strategy can achieve high efficiency with low emissions. However, it has also been revealed that RCCI combustion is difficult at high loads due to its premixed nature. To operate at moderate to high loads with gasoline/diesel dual fuel, high amounts of EGR or an ultra low compression ratio have shown to be required. Considering that both of these approaches inherently lower thermodynamic efficiency, in this study natural gas was utilized as a replacement for gasoline as the low-reactivity fuel. Due to the lower reactivity (i.e., higher octane number) of natural gas compared to gasoline, it was hypothesized to be a better fuel for RCCI combustion, in which a large reactivity gradient between the two fuels is beneficial in controlling the maximum pressure rise rate.

The multi-dimensional CFD code, KIVA3V, was used in conjunction with the CHEMKIN chemistry tool and a Nondominated Sorting Genetic Algorithm (NSGA-II) to perform optimization for a wide range of engine operating conditions. Engine design parameters that were controlled by the genetic algorithm include the fraction of total fuel that is premixed (methane), the timing of the two diesel injections, the amount of diesel in each injection, the diesel fuel injection pressure, and the EGR percentage. The objective of the optimization was to simultaneously minimize soot, NO_x, CO, and UHC emissions, as well as ISFC and ringing intensity. A broad load/speed range was investigated; six operating points from 4 to 23 bar IMEP and 800 to 1800 rev/min were optimized. These load/speed combinations represent typical heavy-duty engine conditions. Using the stock compression ratio of 16.1, it was determined that operation up to 13.5 bar IMEP could be achieved with no EGR, while still maintaining high efficiency and low emissions. The study also examined the sensitivity of RCCI combustion at high load to injection system parameters. The results emphasize that precise injection control is needed for combustion control.

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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 the direct connection to CO₂ emissions and crude oil usage. Hence, the heavy-duty diesel engine has been a topic of research and development over the last two decades.

The emissions consequences of conventional DICI mixing-limited combustion can be best illustrated in terms of equivalence ratio (Φ) and temperature, as shown in [Figure 1](#) [1] where the operating regimes of conventional diesel, PCCI, and HCCI have been overlaid. This figure is based on the original diagram presented by Kamimoto [2] and additional

studies have been performed by Pickett et al. [3], Akihami et al. [4], and others. It can be seen that there are two distinct emissions formation zones: at stoichiometric mixture ($\Phi = 1$), there exists a diffusion flame (i.e., mixing-controlled burning) that yields high NO_x formation rates, and where $2 < \Phi < 3$ with $T \sim 1800$ K, unacceptably high soot formation rates are produced.

In an effort to reduce NO_x and soot emissions while maintaining high thermal efficiency, many new compression ignition (CI) 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 Najt and Foster in 1983 [5]. 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 [6]. In addition, the lean, low temperature combustion process yields near zero NO_x and soot emissions,

as Figure 1 indicates. While HCCI combustion appears thermodynamically attractive, the concept presents a controllability challenge, as it sacrifices two combustion control aspects. First, the timing of ignition is not controlled, either by fuel injection, as in a DICI 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 DICI 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.

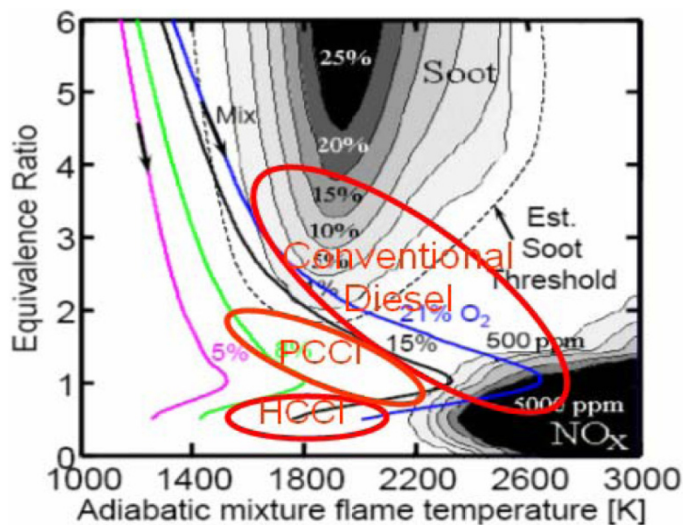


Figure 1. Soot and NOx formation regions in Φ -T space. Overlaid are operating regimes of conventional diesel, premixed charge compression ignition (PCCI), and homogeneous charge compression ignition (HCCI) [1, 2, 3, 4].

To address the first aforementioned combustion control aspect of HCCI combustion, Olsson et al. [7, 8, 9] demonstrated ignition timing control by using two fuels. By using combinations of fuels that possess a large reactivity gradient, proportions between the high- and low-reactivity fuels were adjusted to control combustion phasing and duration. The researchers were able to use combinations of iso-octane (C_8H_{18})/n-heptane (C_7H_{16}) and ethanol (C_2H_6O)/n-heptane, as well as high amounts of EGR to delay the location of 50% fuel burned (CA50). However, the experiments were limited in load due to losses induced by the turbocharger. Exhaust gas temperatures in HCCI are considerably lower than in other combustion strategies, so high levels of boost were unreachable. The experiments resulted in very low NOx, and combustion efficiencies above 95%, especially at mid- to high-load points and when EGR was introduced. However, efficient low-load operation still proved to be a difficult task for HCCI. 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 NOx 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 early 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) [10]. They found that the traditional NOx-soot trade-off present in conventional DICI 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 NOx 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 to accomplish PPCI combustion is to use low-reactivity fuels to allow for more mixing time before ignition. Kalghatgi [11] was one of the first to operate a heavy-duty compression ignition engine with conventional gasoline. More recently, researchers at Lund University have studied gasoline PPCI in a heavy-duty engine from low- to high-load. Manente et al. [12, 13, 14] have developed an operating strategy very similar to UNIBUS [15] to operate a heavy-duty DICI 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 the range of 1-2 FSN, gross indicated efficiency above 50%, NOx below 0.3 g/kW-hr, and maximum pressure rise rates around 15 bar/deg. They were also successful in operating over a large load range (approximately 5-26 bar IMEP) with fuels that had the same boiling point as gasoline. Gross indicated efficiencies were also above 50%, with emissions below US 2010 and EU IV regulations.

A genetic algorithm optimization conducted by Dempsey and Reitz [16] explored gasoline PPCI operation in a heavy-duty compression ignition engine at mid- and high-load with the stock compression ratio of 16.1. The mid-load condition exhibited low emissions, gross indicated thermal efficiency of 50%, and acceptable peak pressure rise rate (PPRR). At the high-load condition, low NOx emissions and an efficiency of 50% were also achieved, but restraining soot and maximum pressure rise rate proved challenging for the gasoline PPCI combustion strategy. This is consistent with the findings of the experimental studies conducted at Lund University that were mentioned previously.

As outlined by Lund University [10,12, 13, 14] and Dempsey et al. [16], single fuel PPCI combustion can yield high thermal efficiency and low emissions, but maintaining an acceptable maximum pressure rise rate is a challenge, especially at high-load. Inagaki et al. [17] were one of the first to demonstrate dual fuel PPCI using in-cylinder fuel blending. They discovered that the ignition timing could be

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.

controlled by changing the ratio of the two fuels and that an injection timing of about 30° before top dead center (BTDC) resulted in combustion rates milder than those exhibited by 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 0.1 FSN (i.e., low soot). Researchers at Lund University [18] were also able to slow the burn rate in HCCI by using two fuels. For example, a mixture of methane and iso-octane was employed to achieve 16 bar IMEP operation at 1000 rev/min. Using a high rate of EGR and relatively late combustion phasing, they were successful in slowing combustion rate and limiting peak cylinder pressures to 17-19 MPa.

Learning from the dual fuel research of Bessonette et al. [19] and Inagaki et al. [17], Kokjohn, Hanson, Splitter, and Reitz [20, 21, 23] 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. [17] could be avoided by using optimized multiple injections with even earlier injection timings than they had used [24]. This allowed them to develop a gasoline/diesel in-cylinder fuel blending strategy that provided low emissions (below US 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. [25], 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. The main focus of the present work was to explore RCCI combustion in a conventional heavy-duty engine from idle to full load (approximately 4-23 bar IMEP) using natural gas as the low-reactivity fuel.

Ignition delay estimates were obtained for various fuels using available chemistry mechanisms and the CHEMKIN code, as shown in Figure 2. It can be seen that the difference in reactivity between methane (CH₄) and n-heptane is much greater than between iso-octane and n-heptane. The larger reactivity gradient aids in extending the combustion duration, thus reducing the peak pressure rise rate at high-load. However, it may pose a challenge at light-load (i.e., the combustion efficiency could suffer). It should be noted that the present study models natural gas as pure methane whereas a typical natural gas contains 92% methane by volume [26], and thus exhibits properties very similar to those of methane. As mentioned previously, the large reactivity gradient between methane and n-heptane makes it attractive for use in

RCCI combustion. Furthermore, natural gas is plentiful. Although more abundant than crude oil, natural gas is still inherently precious and this necessitates the optimization of strategies to burn natural gas efficiently in internal combustion engines.

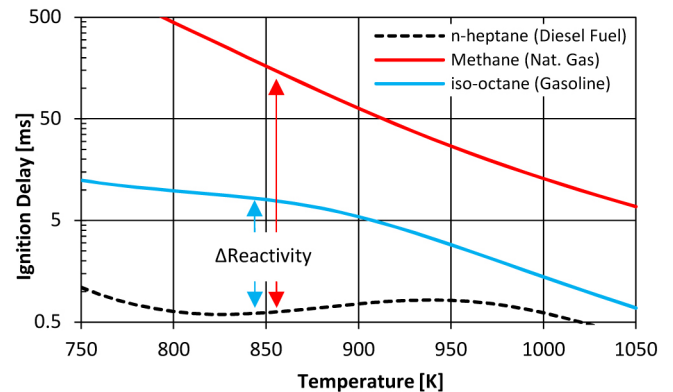


Figure 2. Constant volume, adiabatic, homogeneous reactor simulations of n-heptane (i.e., diesel fuel), methane (i.e., natural gas) and iso-octane (i.e., gasoline). All simulations were conducted at a pressure of 50 bar and an equivalence ratio of 0.4. The location of the delta reactivity line is fairly arbitrary, but 850 to 900 K is a representative compression temperature for heavy-duty diesel engines.

COMPUTATIONAL TOOLS

MULTI-DIMENSIONAL ENGINE CFD

The KIVA-CHEMKIN code, which is based on the KIVA3V Release 2 code [27, 28, 29], was used in this work. The KIVA3V code uses the Lagrangian-Drop Eulerian-Fluid (LDEF) approach for modeling engine sprays: liquid fuel is treated as a Lagrangian parcel and the ambient gas is discretized into cells. The physical properties of natural gas and diesel fuel (for spray break-up, evaporation, and mixing) are taken to be those of methane and tetradecane (C₁₄H₃₀), respectively. It should also be noted that, in this study, the methane and air mixture was assumed to be a homogeneous charge at IVC (i.e., as if the methane was port-injected and had sufficient time to mix with intake air).

Several sub-model improvements have been made to the KIVA3V code, including fuel droplet break-up and evaporation, droplet collision and coalescence, turbulence modeling, grid-independent spray models, and the development of primary reference fuel chemical mechanisms. Beale and Reitz [30] implemented the Kelvin Helmholtz - Raleigh Taylor (KH-RT) model, a hybrid spray break-up model. The original KIVA3V droplet collision model, based on O'Rourke's model, is used. However, a radius of influence (ROI) method was applied to reduce the mesh dependency of the collision process by determining possible collision partners [31]. Droplet-wall interaction was modeled with the

standard KIVA3V wall film model developed by O'Rourke and Amsden [32]. The droplet vaporization sub-model was improved by Ra and Reitz [33]. Furthermore, the RNG k- ϵ turbulence model was modified and implemented into the KIVA3V code by Han and Reitz [34]. To reduce the simulation time, the dynamic maximum timestep strategy developed by Dempsey et al. [16] was used.

The KIVA-CHEMKIN code has been coupled to the CHEMKIN II libraries for detailed combustion chemistry calculations [35]. Soot emissions were predicted using a phenomenological soot model. Two competing processes, formation and oxidation, are considered in the model. Acetylene (C_2H_2) is used as the soot inception species in the formation rate equation [36]. The NO_x formation chemistry is represented by 4 species and 12 reactions, which is a reduced version of the GRI NO_x mechanism [1]. The methane portion of the chemical mechanism used takes into account chain initiation (e.g., $CH_4 + O_2 \rightarrow CH_3 + HO_2$), chain propagating (e.g., $CH_3 + O_2 \rightarrow CH_2O + OH$), and chain branching (e.g., $CH_2O + O_2 \rightarrow HO_2 + HCO$) reactions [37].

OPTIMIZATION METHODOLOGY

Shi and Reitz [38] assessed the performance of different Multi-Objective Genetic Algorithms (MOGA) used in DIC 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 as 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. [39] with a large population size displayed better performance in approaching the true Pareto front and spreading the optimal solutions over all the objectives.

When studying multi-objective problems, trade-offs always exist between designs. For example, an engine design that yields low fuel consumption and low acoustic noise might have high emissions. This raises the question: what defines 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., the objectives) is Pareto optimal if there exists no other solution set that 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 3 [38].

As labeled in Figure 3, letters A through H are solution sets. Solutions A-D are considered Pareto optimal cases because they provide a simultaneous decrease in both objectives, as compared with E-H. This "front" of optimum solutions is commonly 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 the

aforementioned optimization by Dempsey and Reitz [16]. Essentially, when the Pareto front stops advancing towards the origin of Figure 3, the optimization is said to have converged.

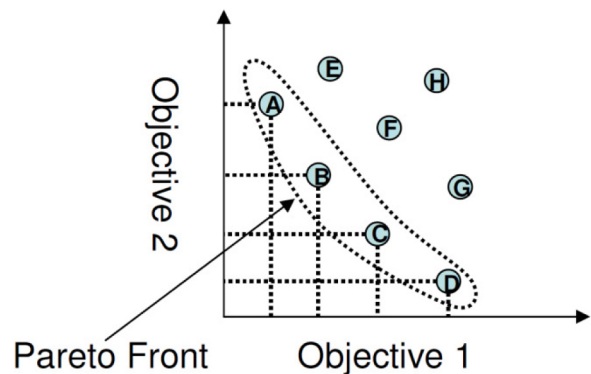


Figure 3. Definition of Pareto optimal "front" in a two objective optimization [38].

Pareto optimality is not the only way to consider an optimum solution to a multi-objective problem. Another common approach is to define cost functions that rank objective importance e.g., if soot is already very low, the optimization might select a citizen with slightly higher soot emission if it had lower NO_x emission. Pareto optimality was used to select optimum strategies in this study, as recommended by Shi and Reitz [38]. Care was taken in cases where certain objectives could be minimized completely (e.g., NO_x and ringing intensity during a misfire). If a citizen misfired, its input parameters were not allowed to be used for further evolution. Therefore, the GA would not pursue certain input parameters that led to misfire (e.g., very high percentage of premixed methane or a very high EGR rate at low-load).

GENETIC ALGORITHM OPTIMIZATION

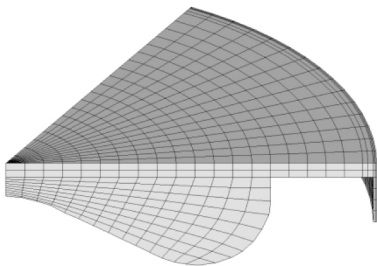
The genetic algorithm optimization was performed on the Caterpillar 3401E Single Cylinder Oil Test Engine (SCOTE) engine geometry. This heavy-duty compression ignition engine utilizes a conventional common rail direct injection system for diesel fuel. The engine and injector specifications are summarized in Table 1.

Table 1. Engine and injector geometry [22].

Caterpillar 3401E SCOTE	
Displacement [L]	2.44
Bore x Stroke [mm]	137.2 x 165.1
Connecting Rod Length [mm]	261.6
Compression Ratio	16.1:1
Swirl Ratio	0.7
IVC [deg ATDC]	-143
EVO [deg ATDC]	130
Common Rail Diesel Fuel Injector	
Number of Holes	6
Hole Diameter [μm]	250
Included Spray Angle [deg]	145

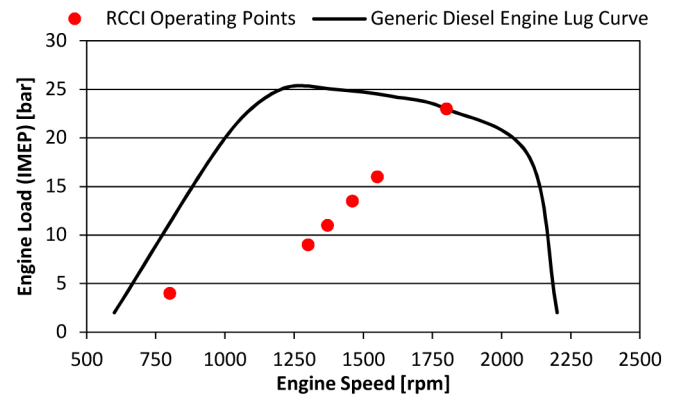
Table 2. Fixed engine operating conditions.

Operating Condition	Low-Load		Mid-Load		High-Load	
Gross IMEP [bar]	4	9	11	13.5	16	23
Engine Speed [rpm]	800	1300	1370	1460	1550	1800
Intake Pressure [bar abs.]	1.00	1.45	1.94	2.16	2.37	3.00
Intake Temperature [$^{\circ}\text{C}$]	60	60	60	60	60	60

**Figure 4. Computational grid used in the optimization (~9500 cells at BDC).**

The three-dimensional computational grid, seen in [Figure 4](#), is a 60-degree sector mesh comprised of approximately 9500 cells at BDC. Run times were generally around 15 hours, and each optimization generation contained 32 citizens. Convergence was typically found after completion of 40 generations.

Dempsey et al. [40] proposed full range operating strategies for gasoline/diesel RCCI combustion using an ultra low compression ratio. These load/speed combinations, which ranged from low-load/low-speed to high-load/high-speed, were selected for the optimization of the present natural gas/diesel operation, as they represent typical heavy-duty engine operating regimes as seen in [Figure 5](#).

**Figure 5. RCCI operating points optimized in this study plotted on a generic lug curve.**

At each condition, the engine speed, fuel energy introduced into the cylinder (i.e., load), and intake pressure were fixed throughout the optimization. These conditions and the corresponding approximate IMEP values are shown in [Table 2](#), while the variable design parameters used in the optimization are listed in [Table 3](#). The objective of the GA was simultaneous minimization of soot, NO_x, CO, and UHC emissions, as well as indicated specific fuel consumption (ISFC) and ringing intensity.