# A Modeling Study of Charge Preparation and Combustion in an HCCI Engine Using a Variable Pressure Pulse (VPP) Injection System and Optimized PRF Blends

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**Abstract**

This study uses a multi-dimensional CFD code, the KIVA-CHEMKIN code, to investigate the use of gasoline/diesel dual fuel blends in an HCCI engine. The detailed chemistry calculations used a primary reference fuel mechanism, which has been extensively validated against experimental data at conditions similar to those of the present study. Parameter optimization was performed by coupling the Non-Dominated Sorting Genetic Algorithm (NSGAII) with the KIVA-CHEMKIN code.

The first part of the study focused on choosing an optimized fuel blend and EGR combination for HCCI operation at two engine loads (6 and 11 bar IMEP). It was found that the minimum ISFC could not be achieved with either neat diesel fuel or neat gasoline. Next, a genetic algorithm (GA) was used with CFD modeling to optimize injection parameters of a split injection event (injection pressures, timings, and fuel split) in order to achieve an adequately homogeneous fuel blend with minimum wall film using port fuel injection of gasoline and direct injection of diesel fuel. Finally, the optimized fuel, EGR, and injection parameters were evaluated with the KIVA-CHEMKIN code and controlled HCCI operation was achieved at 11 bar IMEP. The optimized fuel blend and EGR rate for 11 bar IMEP were PRF 65 and 50%, respectively. The injection optimization resulted in 64% of the diesel fuel being injected at 67° BTDC with an injection pressure of 100 bar. The remainder of the fuel was injected at 33° BTDC at 550 bar. The combination of optimized fuel, EGR, and injection parameters resulted in near zero NOx and soot and a net ISFC of only 163 g/kW-hr.

## Introduction

Many researchers have shown that premixed compression ignition combustion (PCCI and HCCI) strategies are capable of achieving low NOx and soot emissions while maintaining diesel like efficiency. Due to the existing fuel infrastructure, most HCCI research has been conducted using either strictly gasoline or diesel fuel. However, in their neat forms, each fuel has specific advantages and shortcomings for HCCI operation. Gasoline has a high volatility; thus, evaporation is rapid and a premixed charge can be obtained using port fuel injection. However, because the autoignition qualities of gasoline are poor, it becomes difficult to achieve combustion at low-load conditions (e.g., [1, 2]). Conversely, diesel fuel has superior auto-ignition qualities; however, this can result in difficulty controlling the combustion phasing as engine load is increased. Furthermore, because diesel fuel is difficult to vaporize, port fuel injection cannot be used and charge preparation becomes a challenge.

Recent experiments performed by Bessonette et al. [3] have suggested that the best fuel for HCCI operation may have autoignition qualities between that of diesel fuel and gasoline. Using a compression ratio of 12:1 and a fuel with a derived cetane number of ~27 (i.e., a gasoline boiling range fuel with an octane number of 80.7), they were able to extend the HCCI operating range to 16 bar BMEP – a 60% increase in the maximum achievable load compared to operation using traditional diesel fuel. Furthermore, their results showed low load operation, below 2 bar BMEP, required a derived cetane number of ~45 (i.e., traditional diesel fuel). Thus, it may be beneficial to explore HCCI operation using fuel blends optimized for specific operating conditions.

This work considers blends of iso-octane and n-heptane (i.e., PRF blends) to simulate the use of gasoline and diesel fuel blends. Based on the work of Bessonette et al. [3], it is likely that different fuel blends will be required at different operating conditions (e.g., a high cetane fuel at light load and a low cetane fuel at high load). Thus, it is desirable to have the capability to operate with fuel blends covering the spectrum from neat gasoline to neat diesel fuel depending on the operating regime. This work proposes port fuel injection of the highly volatile gasoline fuel and early cycle direct injection of diesel fuel. To address the spray wall impingement issue associated with early

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cycle injections, a variable pressure pulse (VPP) injection system was developed in the Diesel Emissions Reduction Consortium (DERC) laboratory at the University of Wisconsin – Madison. This system is described by Kokjohn et al. [4] and is capable of delivering multiple injections pulses at different injection pressures in the same engine cycle. Sun et al. [5] and Kokjohn et al. [4] have shown the advantages of using low-pressure injections with a fixed spray angle as a means for reducing spray wall impingement for early injected fuel.

**Materials and Methods**

The engine modeled in this study is a Caterpillar 3401 E Single Cylinder Oil Test Engine (SCOTE) and the injector is a high-pressure common rail type manufactured by Bosch. Engine and injector specifications are given in Table 1. Two operating conditions are considered in the present work, 1300 rev/min and 6 bar IMEP, and 1300 rev/min and 11 bar IMEP.

To determine the optimal fuel blend and EGR rate for the spray studies, a single zone engine model was developed using the Senkin [6] combustion package and a reduced PRF mechanism [7]. The reduced PRF mechanism has been extensively validated against experimental data at conditions similar to those of the present study [7]. To account for wall heat transfer, the modified Woschni correlation of Chang et al. [8] was used. The multi-dimensional spray and combustion computations were performed using the KIVA-3v release 2 code [9] coupled with the CHEMKIN II solver and the reduced PRF mechanism [7]. Since the introduction of KIVA, many physical and chemistry models have been developed at the University of Wisconsin – Madison's Engine Research Center (ERC). The spray model used the grid independent gasjet model of Abani et al. [10] and the KH-RT breakup model [11]. Droplet collision is predicted using a radius of influence approach, as suggested by Munnannur [12].

**Table 1.** Engine and injector specifications

| | |
|---|---|
| Base engine type | 2.44 L CAT SCOTE |
| Bore x stroke | 13.7 x 16.5 cm |
| Connecting Rod Length | 26.1 cm |
| Squish height | 0.157 cm |
| Geometric compression ratio | 16.1:1 |
| Swirl ratio | 0.7 |
| Bowl type | "Mexican Hat" |
| Intake valve closing (IVC) | -95º ATDC Firing |
| Exhaust valve opening (EVO) | 130º ATDC Firing |
| Injector | Bosch common rail 6 x 250 μm |
| Included angle | 145° |

**Results and Discussion**

The single zone engine code was used to select an optimal fuel blend and EGR rate to achieve HCCI combustion. The operating conditions for each load point are given in Table 2. A homogeneous mixture of the specified PRF blend (defined as the molar fraction of iso-octane in the fuel) was assumed at intake valve closure (IVC) and simulations were run from IVC to EVO. The design space was populated by varying EGR in increments of 5% from 0% to 70% and the PRF number in increments of 5 from 0 (neat n-heptane) to 100 (neat iso-octane).

**Table 2.** Operating conditions of the single zone combustion study

| Engine Speed (rev/min) | IMEP (bar) | IVC timing (° aTDC) | IVC pressure (bar) | IVC temperature (K) | Fuel rate (mg/cycle) |
|---|---|---|---|---|---|
| 1300 | 6 | -95 | 2.10 | 367 | 67.5 |
| 1300 | 11 | -95 | 3.18 | 367 | 135 |

Figure 1 shows the predicted effect of EGR rate and PRF number on net ISFC at each load point. The stars indicate the operating points with an ISFC below 180 g/kW-hr and a peak pressure rise rate (PRR) below 30 bar/deg. Note that this upper limit of pressure rise rate was suggested by Bessonette et al. [3] as a hard limit for a heavy-duty diesel engine. Furthermore, it must be noted that comparisons with experimental data (not presented here for brevity) showed that the single zone model over predicts the peak pressure rise rate due to the assumption of a spatially homogeneous mixture and temperature. Thus, it is likely that more points would meet the pressure rise rate constraint if inhomogeneity in temperature and mixture distribution were considered.

Several observations can be made from the results presented in Fig. 1. At the 6 bar IMEP operating point a PRF number of ~60 is required to achieve the minimum ISFC, that is, the minimum fuel consumption point cannot be

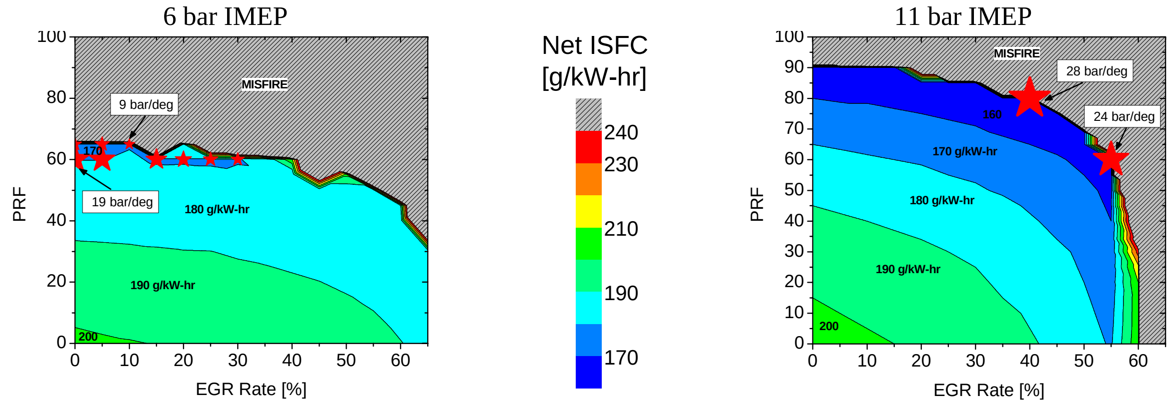



**Figure 1.** Effect of PRF and EGR on fuel consumption. The red stars indicate cases with peak pressure rise rates below 30 bar/deg. and net ISFC below 180 g/kW-hr.

achieved with either neat n-heptane or neat iso-octane. Lower PRF blends resulted in advanced combustion phasing and increased compression work, while higher PRF blends delayed combustion phasing and significantly reduced combustion efficiency. Note also the very sharp boundary between highly efficient and misfire operation.

As the load is increased to 11 bar IMEP, the contours shift toward higher PRF numbers in order to phase combustion after TDC. The contours of Fig. 1 show that very low ISFC (~160 g/kW-hr) can be achieved using PRF blends ranging from 45 to 90 depending on the EGR level. It is again found that the minimum ISFC cannot be achieved with neat diesel fuel or gasoline. Furthermore, as the load is increased, operation must be shifted to higher EGR levels in order to reduce the rate of heat release and meet the peak pressure rise rate constraint.

The single zone combustion study indicated that it is possible to improve fuel economy by optimizing the PRF blend for a specific operating condition. Accordingly, the next phase of the work focused on achieving a desired PRF blend by port fuel injection of gasoline and direct injection of diesel fuel. The 11 bar IMEP operating point was selected for the charge preparation study and a PRF number of 65 was used (i.e., 88 mg of gasoline was premixed and 47 mg of diesel fuel was direct-injected using the injector of Table 1). The KIVA-3v release 2 code was used for the spray simulations and was coupled with a multi-objective genetic algorithm (MOGA) for parameter optimization. Details of the MOGA optimization strategy can be found in Kokjohn et al. [4, 13]. The charge preparation optimization considers only spray and mixing, that is, chemistry is not solved. Calculations were run from IVC to 10 °BTDC (near ignition). To evaluate the effectiveness of each design, wall film levels and PRF number inhomogeneity were compared. The PRF number inhomogeneity is a mass weighted sum of the squared difference between the local (cell) and global PRF number and is defined as

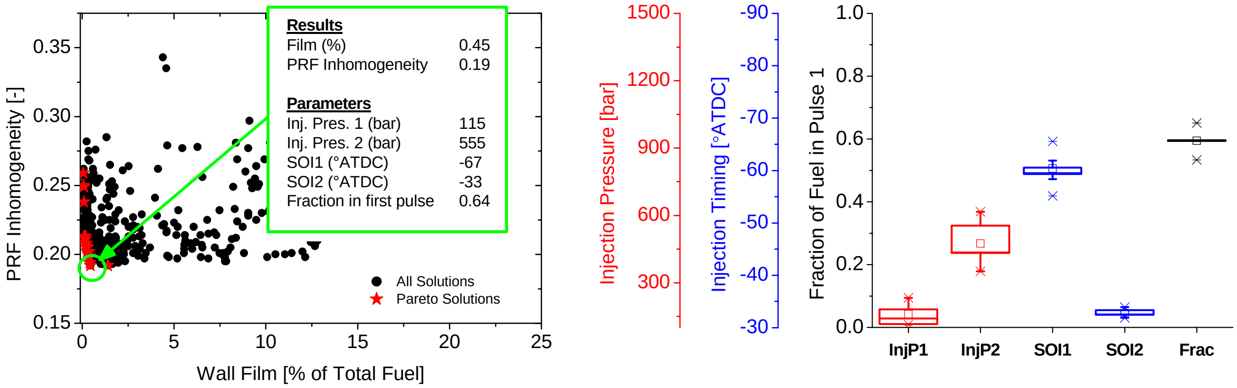
$$NSD_{PRF} = \sqrt{\frac{\sum_{i=1}^{ncells}\left(m_i\left(PRF_i - PRF_{GLOBAL}\right)^2\right)}{PRF_{GLOBAL}\sum_{i=1}^{ncells} m_i}} \tag{1}$$

where $PRF_i$ and $m_i$ are the fuel PRF number and mass in each computational cell. $PRF_{GLOBAL}$ is the overall PRF number for the entire combustion chamber.

Table 3 shows the parameters and ranges of the charge preparation optimization study. The results of the optimization are shown in Fig. 2 (a). A case with minimum PRF inhomogeneity and very low wall film was selected for further analysis. The parameters of the selected case are representative of the Pareto solutions (see the box plot of Fig. 2 (b)). Generally, the Pareto solutions used a low pressure (100 to 200 bar) first injection between 57 and 70 °BTDC with ~60% of the diesel fuel followed by a higher pressure (350 to 600 bar) second injection near 33 °BTDC.

**Table 3.** Optimization parameters

| | |
|---|---|
| First pulse injection timing (SOI1) | IVC to (SOI2 – 20°) |
| Second pulse injection timing (SOI2) | -50 to -30 °ATDC |
| First pulse injection pressure (InjP1) | 100 to 1500 bar |
| Second pulse injection pressure (InjP2) | 100 to 1500 bar |
| Fraction of fuel in the first pulse (frac) | 0 to 1 |




**(a)** **(b)**

**Figure 2. (a)** Charge preparation optimization results. The stars indicate Pareto solutions and the case selected for further analysis is designated with a circle. The results and parameters of the selected Pareto solution are also shown. **(b)** Box plot showing the distribution of parameters for the Pareto solutions.

The COmponent Selection and Smoothing Operator (COSSO) [14, 15] technique was used to provide a quantitative interpretation of the effect of each design parameter. Using the COSSO technique with the selected design of Fig. 2**.** as the center point, it was found that PRF inhomogeneity is mainly influenced by the fuel split and first pulse injection timing. Figure 3 shows the response surface of PRF inhomogeneity as a function of fuel split and first injection timing. These two parameters influence the distribution of the injected fuel, that is, the split of fuel between the piston bowl and squish regions. To create a homogeneous charge the fuel must be optimally distributed between these two regions of the combustion chamber; thus, it is reasonable that fuel split and first pulse injection timing are key factors to minimize PRF inhomogeneity. Furthermore, it can be concluded that the choice of the range of second injection timing is responsible for the small impact of second injection timing on PRF inhomogeneity. Specifically, for the allowed second injection timings, the spray targeting is such that the majority of the fuel is directed into the piston bowl.

The response surfaces for fuel film suggest there are three controlling factors for wall film levels: first pulse injection pressure, first pulse injection timing, and fuel split. Key response surfaces are also shown in Fig. 3. Because early cycle charge densities are low, long liquid lengths are observed and controlling the targeting and spray penetration becomes important. Consequently, the parameters of the first injection have the largest influence on fuel film levels. In this work it is shown that appropriately combining, fuel split, injection pressure, and injection timing is essential to minimize wall film levels. The response surface comparing the effects of first and second pulse injection pressure suggest that low pressure injections are most effective at minimizing wall film for injection timings earlier than 50 °BTDC.

To complete the present study, the results of the spray optimization were extended to a closed cycle combustion analysis. The KIVA-3v release 2 code coupled with the CHEMKIN II solver and a reduced PRF mechanism [7] was used to simulate the spray and combustion events. Table 4 shows the parameters and results of the selected case of Fig. 2. As can be seen, HCCI operation at an IMEP of 11 bar is achieved with near zero NOx and soot and extremely low net ISFC. The net ISFC was calculated using the simulated pressure trace combined with the pumping loop obtained from experimental data. The very low ISFC is the result of optimal combustion phasing (minimizing

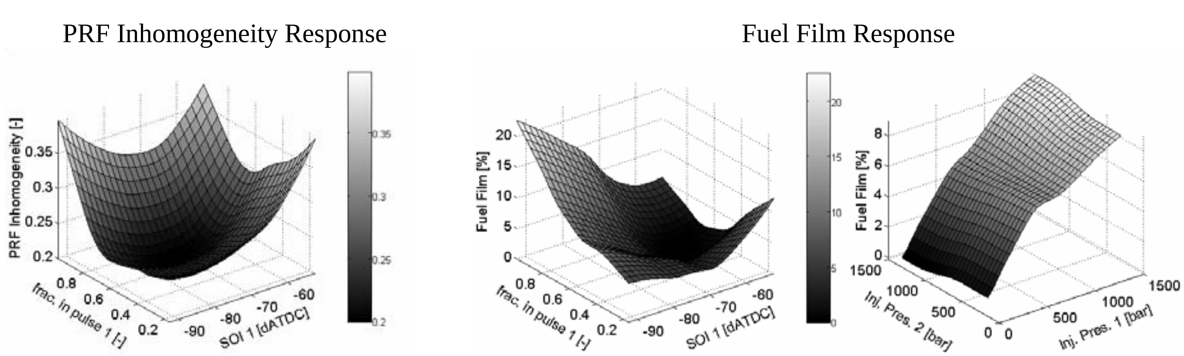



**Figure 3.** Response surfaces for PRF inhomogeneity and fuel film generated using the COSSO [14] technique.

compression work and maximizing expansion work) through the use of the optimized fuel blend. Figure 4 shows representative in-cylinder images of the spray and combustion events and Fig. 5 shows the calculated cylinder pressure and heat release rate. Note that the first injection targets the squish region and the second injection targets the bowl in order to provide a well mixed fuel blend by the onset of heat release. The temperature contours show that heat release initiates in the region where the lowest PRF number is observed, as expected, and is subsequently followed by volumetric heat release throughout the chamber. The n-heptane and iso-octane contours show that nearly all of the n-heptane is consumed prior to consumption of iso-octane. The staged consumption of n-heptane and iso-octane results in an extended heat release duration, as seen in Fig. 5, and thus results in a reasonable rate of pressure rise at 11 bar IMEP.

**Table 4.** Parameters and results of spray and combustion study at 11 bar IMEP and 1300 rev/min.

| Parameters | | | | | | | Results | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| PRF (-) | EGR (%) | Inj. P1 (bar) | Inj. P2 (bar) | SOI 1 (°ATDC) | SOI 2 (°ATDC) | Fract. (-) | NOx (g/kgf) | Soot (g/kgf) | HC (g/kgf) | CO (g/kgf) | PRR (bar/deg.) | ISFC (g/kW-hr) |
| 65 | 50 | 115 | 555 | -67 | -33 | 0.64 | 0.2 | 0.002 | 2.0 | 6.0 | 12.9 | 163 |

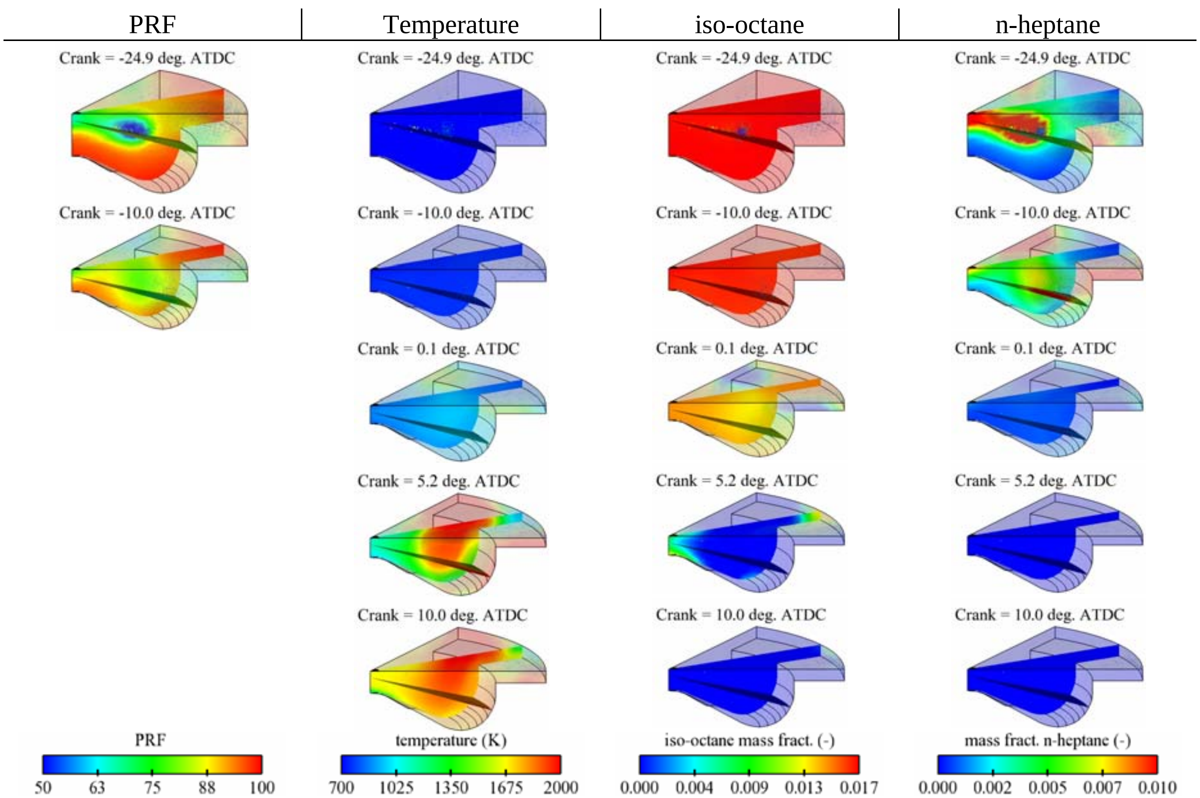



**Figure 4.** Spray and combustion images of in-cylinder PRF number, temperature, mass fraction of iso-octane, and mass fraction of n-heptane on cut planes coincident with the spray axis. Note that the PRF number is undefined after the start of combustion; thus, images are not presented after the onset of significant heat release.

## Conclusions

This study has investigated the use of dual fuel blending as a means to extend the load limit of HCCI operation. Blends of gasoline (iso-octane) and diesel fuel (n-heptane) were used to provide optimal auto-ignition qualities. A single zone engine model was used to determine the best fuel blend and EGR rate for two engine loads (6 and 11 bar IMEP). The results of the single zone combustion investigation showed that the minimum ISFC cannot be achieved with either neat diesel fuel or neat gasoline; furthermore, it was found that as load was increased higher PRF blends were required to phase combustion appropriately.

A multi-objective genetic algorithm optimization was performed next to optimize the parameters of a split injection in order to achieve a spatially homogeneous fuel blend with minimum wall film using port fuel injection of gasoline and direct injection of diesel fuel. The results of the optimization were analyzed using the COSSO technique and it was found that the most important parameters for reducing PRF inhomogeneity were the fuel split amounts and first pulse injection timing. These parameters were found to be influential in controlling the fuel distribution, thus minimizing PRF inhomogeneity. Furthermore, it was shown that near zero wall film levels can be achieved with optimized fuel split, low first pulse injection pressure, and appropriate injection timing.

The single zone combustion modeling and spray optimization results were then combined and multi-dimensional spray and combustion CFD calculations were performed. It was found that through the optimal combination of EGR, fuel reactivity, and injection parameters, well controlled HCCI combustion could be achieved at an intermediate load of 11 bar IMEP with near zero NOx and soot and a net ISFC of only 163 g/kW-hr.

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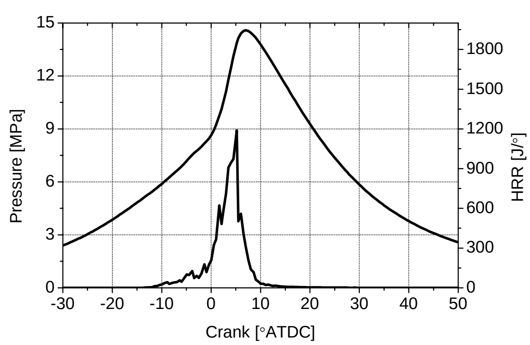


**Figure 5.** Calculated cylinder pressure and heat release rate for optimum case (see Table 4).