

A Computational Investigation of Two-Stage Combustion in a Light-Duty Engine

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ABSTRACT

The objective of this investigation is to optimize light-duty diesel engine operating parameters using Adaptive Injection Strategies (AIS) for optimal fuel preparation. A multi-dimensional Computational Fluid Dynamics (CFD) code with detailed chemistry, the KIVA-CHEMKIN code, is employed and a Multi-Objective Genetic Algorithm (MOGA) is used to study a Two-Stage Combustion (TSC) concept. The combustion process is considered at a light load operating condition (nominal IMEP of 5.5 bar and high speed (2000 rev/min)), and two combustion modes are combined in this concept. The first stage is ideally Homogeneous Charge Compression Ignition (HCCI) combustion and the second stage is diffusion combustion under high temperature and low oxygen concentration conditions. Available experimental data on a 1.9L single-cylinder research engine is used for model validation. The results show that the computations are able to adequately predict the emissions trends and quantities over an injection timing sweep for the Partially Premixed Compression Ignition (PCCI) cases investigated. A preliminary investigation was performed to gain an understanding of two-stage combustion in the light duty engine. At this condition it was found that pure HCCI combustion could yield very low engine out emissions, but extreme pressure rise rates would lead to excessive combustion noise. A multi-dimensional optimization code, NSGAII, was used for optimization of six objectives (NO_x, soot, CO, HC, ISFC, and peak PRR) by adjusting four parameters (boost pressure, EGR rate, fraction of premixed fuel, and start of late injection timing). The optimization has shown that two-stage combustion is a feasible concept for noise reduction while maintaining reasonable emissions and fuel consumption. A Pareto solution yielding a peak pressure rise rate of 4.3 bar/deg was found using a high EGR rate (54%), relatively low IVC pressure (1.74 bar), premixing 36% of the total fuel, and injecting the remainder of the fuel at 2.9 degrees after TDC.

INTRODUCTION

Since its introduction in the late 1800's, the diesel engine has been utilized in almost every aspect of modern life, from transportation to energy generation to food production. Several emissions are of prime concern for air pollution: nitrogen oxides (NO_x), carbon monoxide (CO), unburned hydrocarbons (HC), and particulates (soot). These pollutants are damaging to the environment and human health. Reduction of these harmful pollutants while maintaining fuel economy has been a primary driving factor for internal combustion engine research in recent years.

Homogeneous Charge Compression Ignition (HCCI) and Premixed Charge Compression Ignition (PCCI) concepts have been shown to be promising techniques for simultaneous NO_x and soot reduction [1-3]. Premixed combustion utilizes a long ignition delay in order to allow adequate time for mixing prior to the start of combustion. Because the fuel and air are well mixed prior to the start of combustion, local rich regions are avoided and very low soot levels are realized. At light load conditions, very high levels of EGR can be employed in order to maintain temperatures below the NO formation region. Relying on Pickett et al. [4] and Akihama et al. [5], Sun [6] has shown the PCCI, HCCI, and traditional diesel

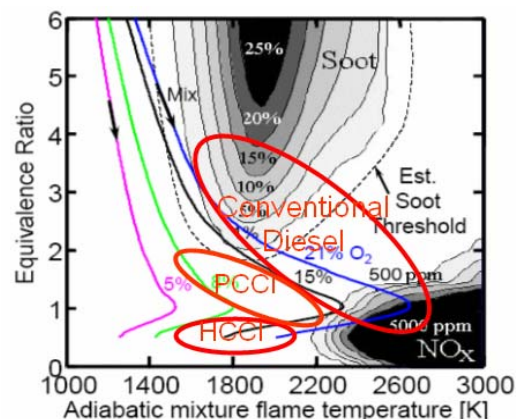


Figure 1. PCCI, HCCI, and conventional diesel operating regimes shown in Φ -T space [6]

operating regimes in the Φ -T space originally presented by Kamimoto [7], see Figure 1.

Although, HCCI and PCCI combustion have been shown to yield very low NO_x and soot levels, these strategies tend to produce high rates of pressure rise and therefore can result in higher combustion noise than conventional diesel operation.. Because noise generated during the combustion process is major concern for light-duty engines, it is desirable to explore concepts that yield the low emissions and high efficiency characteristics of premixed combustion, while maintaining acceptable pressure rise rates.

Hasegawa and Yanagihara [8] explained the Uniform Bulky Combustion System (UNIBUS) which involves a dual injection strategy. An early injection well before TDC creates a premixed charge. Engine parameters (intake gas temperature, boost pressure, fuel quantity, and injection timing) are set such that high temperature heat release does not occur prior to the start of late injection. The second injection occurs after TDC and is used to control the start of combustion of the premixed fuel. They found that after the late injection, combustion occurred at many points simultaneously throughout the chamber; thus suggesting HCCI combustion was achieved. The UNIBUS concept was able to achieve low NO_x and near-zero soot emissions

Sun [6, 9] has shown the possibility of emissions reduction using a Two-Stage Combustion (TSC) concept in a heavy-duty diesel engine. The TSC strategy is similar to the UNIBUS concept; however Sun's strategy uses higher quantities of fuel injected early in the cycle to result in two distinct heat release events. The first stage is HCCI-like combustion and the second stage is diffusion combustion under low oxygen concentration conditions. Note that in this paper the terminology 'cool flame reaction' describes the low temperature reaction associated with forming a pool of hydrogen peroxide which will later be consumed in the high temperature reaction, 'First stage combustion' refers to high temperature heat release of an early injected or premixed fuel, and 'second stage combustion' refers to combustion of a late injected fuel. Because in the TSC strategy only a fraction of the total fuel is burnt in pure HCCI combustion it may be possible to use the TSC concept for noise reduction. This study aims to apply the TSC concept to a light-duty diesel engine in order to minimize pollutant emissions and to improve fuel economy while maintaining low engine noise.

A multi-dimensional CFD code with detailed chemistry, the KIVA-CHEMKIN code, was employed in this investigation. Model validation was performed using experimental data of Opat et al. [3]. After the model validation, a preliminary investigation was performed to gain a basic understanding of the two-stage combustion concept in a light-duty diesel engine. With a basic understanding of two-stage combustion, a multi-objective genetic algorithm (MOGA) was used to optimize engine parameters to minimize pollutants, engine noise, and fuel consumption.

COMPUTATIONAL MODEL

Computations were performed using the KIVA-3v release 2 code [10] with improvements to many physical and chemistry models developed at the ERC [11-15]. The KIVA-3v code was coupled with the CHEMKIN II solver for detailed chemistry calculations. A 34 species and 77 reaction mechanism for n-heptane [16] (see Appendix A) was used to simulate diesel fuel chemistry.

Droplet breakup was modeled using a hybrid Kelvin Helmholtz (KH) – Rayleigh Taylor (RT) model [13]. Gasjet theory was employed to model the relative velocity between the droplets and gas phase in the near nozzle region in order to reduce grid dependency [11, 12]. Turbulence was modeled using the RNG k- ϵ model [14]. An unsteady droplet vaporization model considering droplet temperatures ranging from flash boiling to normal evaporation was employed [15]. The droplet collision model is based on O'Rourke's model; however, a radius of influence method is used to determine the possible collision partners to further remove mesh dependency [11]. Droplet interactions with the wall were considered through a wall film submodel [17, 18] which included the effects associated with splash, film spreading, and motion due to inertia. Soot was predicted using a phenomenological soot model [19] based on the model of Hiroyasu [20]. The soot model used in the present study used acetylene as an inception species, which allows the soot model to be coupled to the chemistry solver through the addition of 13 reactions involving acetylene. NO_x emissions were predicted using a reduced NO mechanism [6] consisting of 4 additional species and 12 reactions. The reduced NO mechanism is based on the Gas Research Institute (GRI) NO mechanism [21]. The reduced NO mechanism described by Sun [6] is shown below:



Parameter optimization was performed using a multi-objective genetic algorithm (MOGA). Shi [22] has shown that the Nondominated Sorting Genetic Algorithm (NSGAI) proposed by Deb et al. [23] performs well in engine optimizations; therefore, NSGAI was selected as

the optimization tool for this study. A multi-objective approach was favored over the use of a merit function based single-objective optimization scheme in order to generate a set of solutions from which the engine designer may choose an in-cylinder strategy which best accompanies the available aftertreatment system.

Sun [6] showed that by utilizing injection timings prior to IVC combined with low-pressure early injection a homogeneous charge could be created with minimal wall-film. Furthermore, he showed that using a homogenous assumption at IVC yielded similar results to modeling the early injection process. Because modeling of the early injection process requires the use of a full cylinder mesh with valve motion which would result in excessively long computational times, the early injection was not modeled; instead it was assumed that a perfectly homogeneous charge had been created at IVC. The computational grid used in this study was a 51.4° sector mesh which represents a single nozzle hole of the 7-hole Bosch injector used in the engine. Abani et al. [12] have shown the improved spray models used in this study yield similar results on both fine and coarse grids. Therefore, in order to reduce computational expense, the rather coarse mesh of Figure 2 was used.

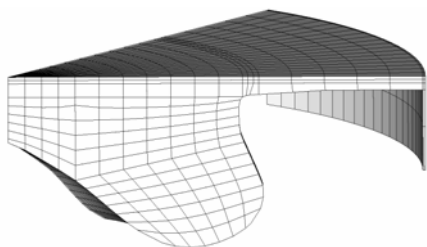


Figure 2. Computational grid with crevice volume, shown at TDC. The grid is a 51.4 degree sector consisting of 11,000 cells at BDC.

ENGINE SPECIFICATIONS

The engine used in this study was a single cylinder version of the GM 1.9 L engine with specifications given in Table 1.

Table 1. engine specifications

Base engine type	GM1.9 L [†]
Bore	8.2 cm
Stroke	9.04 cm
Connecting Rod Length	16.1 cm
Squish height	0.0617 cm
Displacement	0.4774 L
Compression ratio	16.5:1
Swirl ratio	2.2
Bowl type	reentrant
Intake valve opening	344° ATDC Firing
Intake valve closing	-132° ATDC Firing
Exhaust valve opening	112° ATDC Firing
Exhaust valve closing	388° ATDC Firing

[†]A single cylinder version of the GM 1.9L engine was used

Table 2. Injector specifications

Injector type	High-pressure common-rail
Manufacturer	Bosch
Injection pressure	860 bar
Included angle	155°
Number of holes	7
Nozzle hole diameter	141 μm

Table 3. Operating conditions for model validation

Engine speed	2000 rpm
IMEP	5.5 bar
Fuel flow rate	0.895 kg/hr
Inlet oxygen concentration	9.5 %
Average equivalence ratio	0.90
IVC temperature	350 K
IVC pressure	1.91 bar

MODEL VALIDATION

Engine experiments performed by Opat et al. [3] were used for computational model validation. The experiments were conducted using a single injection PCCI approach at the same operating condition investigated in the present study (5.5 bar nominal IMEP and 2000 rev/min). To achieve PCCI combustion, Opat utilized an early injection (~30 °bTDC) to attain adequate mixing prior to the start of combustion and a high EGR rate (~65%) to suppress in-cylinder temperatures and increase ignition delay. Model validation was performed over a start of injection (SOI) sweep from 34.2 to 16.2 deg before TDC. Figure 3 shows the cylinder pressure and heat release rate comparison from a representative case with an SOI of 29.2 degrees before TDC. The locations of the cool flame and main heat release are predicted very accurately; however, the simulation predicts slightly higher cylinder pressure than the experiment. This difference in cylinder pressure can be attributed to an over-prediction of the evaporation process during the injection event for this condition. In addition, the simulation predicts two peaks on the high temperature heat release, which is not observed in the experiments. The two-peak behavior is explained by competition for OH radicals between the $\text{CO} + \text{OH} \rightarrow \text{CO}_2 + \text{H}$ reaction and other less exothermic reactions. As OH radicals are consumed by reactions other than the $\text{CO} + \text{OH} \rightarrow \text{CO}_2 + \text{H}$ reaction the high temperature heat release slows down. Meanwhile, CO continues to accumulate and is finally consumed when a sufficient pool of OH radicals are formed through chain branching reactions. The two-peak behavior can be eliminated by adjusting the rates of the competing reactions; however, the current n-heptane mechanism generally performs better under low temperature combustion conditions than the modified version [24].

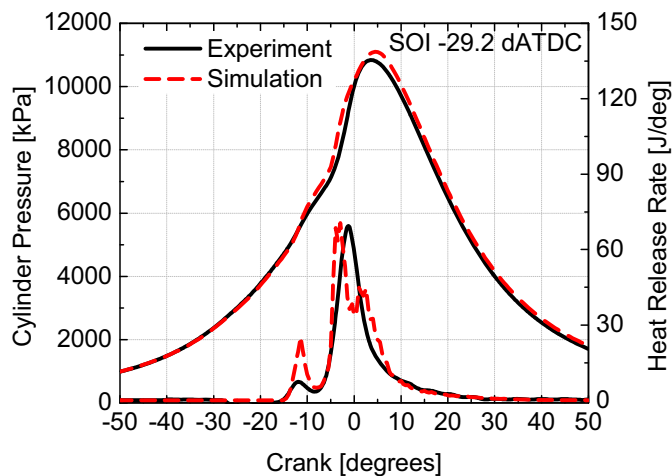


Figure 3. Comparisons of computed and measured cylinder pressure and heat release rate. The start of injection was 29.2 degrees before TDC.

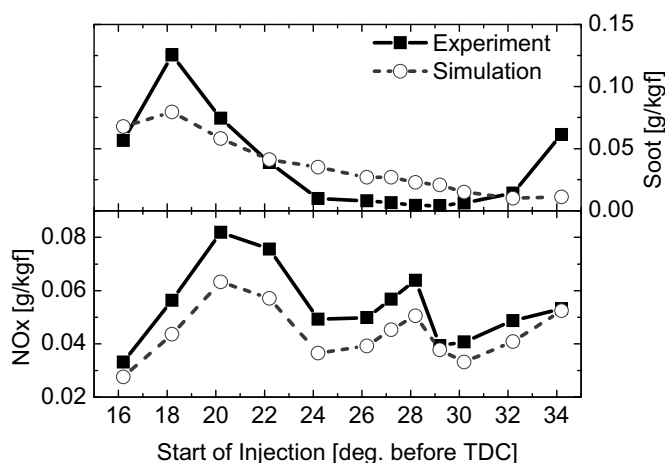


Figure 4. Engine-out NOx and Soot emissions computed by KIVA compared with measured values over an injection timing sweep.

Figure 4 shows comparisons of predicted and measured soot and NOx emissions. The simulation soot results do not show as much sensitivity to start-of-injection timing as the experimental data. Nevertheless, the soot trend is predicted reasonably well for all but the earliest injection timings. At an SOI of 34 degrees before TDC the experiments show a sharp increase in soot levels; however, the simulation results show a flattening out of the soot versus SOI curve. The simulation captures all of the NOx trends exhibited by the experimental data; however the results show the simulation slightly under predicts NOx for all injection timings.

Figure 5 shows comparisons of measured and predicted CO and HC emissions. The CO trend shows good agreement for injection timings later than 28.2 degrees before TDC. As SOI is further advanced the experimental data shows an increase in CO levels while the simulation shows a flattening off and then a decrease in CO levels. Significant wall impingement is observed as the SOI is advanced beyond 30 degrees before TDC. Therefore, the discrepancy between the

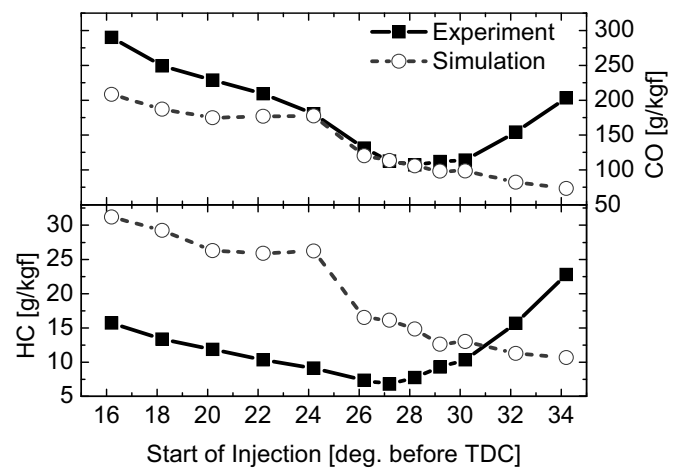


Figure 5. Engine-out HC and CO emissions computed by KIVA compared with measured values over an injection timing sweep.

simulation and experimental results may be due to limitations of the wall film model. Because the present investigations were primarily concerned with cases with little wall film, this discrepancy is not likely to significantly impact the results of this study. HC emissions are over-predicted for a majority of the injection timings considered, thus suggesting that the model will provide a conservative prediction of the HC emissions. Similar to CO, a discrepancy between simulation and experimental HC trends becomes present as the SOI is advanced to very early injection timings.

RESULTS AND DISCUSSION

This section consists of three parts. In the first part an investigation is performed to determine if two-stage combustion is a feasible means of lowering combustion noise while maintaining reasonable emissions. In the second part a multi-objective genetic algorithm is employed to optimize engine parameters in a two-stage combustion operating condition. In the third part a parametric study is conducted to investigate the effects of IVC pressure, EGR rate, premixed fuel fraction, and late injection timing on emissions, fuel consumption, and engine noise on a selected Pareto solution.

PRELIMINARY INVESTIGATION

A preliminary investigation was performed to gain an understanding of two-stage combustion in the present light-duty diesel engine. IVC pressure, IVC timing, EGR, start-of-late-injection timing (SOLI), and total fueling were held constant at 1.91 bar, 132 °BTDC, 0 %, top dead center, and 0.895 kg/hr respectively. The fraction of fuel participating in HCCI combustion was varied from 0% (diesel combustion) to 100% (pure HCCI combustion). Fuel fraction, premixed fuel mass, injected fuel mass, the duration of the late injection, and equivalence ratio of the premixed fuel are shown in Table 5.

Table 4. Preliminary investigation operating conditions.

Engine speed.....	2000 rpm
IMEP.....	5.5 bar
Total fuel quantity.....	14.9 mg/stroke
Late injection timing.....	TDC
Inlet oxygen concentration.....	21 %
Average equivalence ratio	0.26
IVC temperature	350 K
IVC pressure	1.91 bar

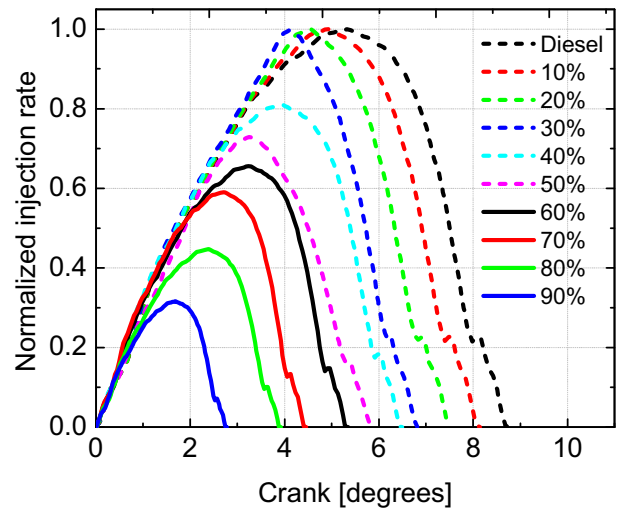
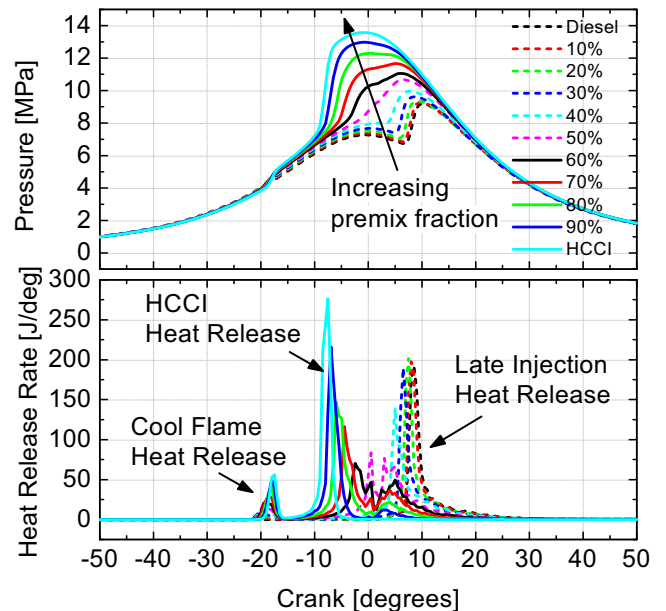
Table 5. Fuel quantities and late injection duration.

Premixed fuel (%)	Premix mass (g)	Injected mass (g)	Inj. dur. (CA _d)	Premixed phi (-)
100	0.0149	0	0	0.26
90	0.01341	0.00149	2.769	0.24
80	0.01192	0.00298	3.916	0.21
70	0.01043	0.00447	4.447	0.18
60	0.00894	0.00596	5.336	0.16
50	0.00745	0.00745	5.415	0.13
40	0.00596	0.00894	6.49	0.11
30	0.00447	0.01043	6.807	0.079
20	0.00298	0.01192	7.515	0.052
10	0.00149	0.01341	8.137	0.026
0	0	0.0149	8.763	0

Juneja [25] has shown that the shape of the rising and falling portions of the injection profile can have a significant impact on pollutant emissions. To yield the most realistic results, it was desirable to use an experimentally derived injection profile for this study and future optimizations. The injection rate for each pulse was scaled from the experimental injection profile presented by Opat [2] such that the rising and falling portions of the injection profile had the same slopes as those given by the experiment. Fuel quantity was adjusted by changing the duration that the injection rate was relatively constant. For very low fueling quantities it was necessary to shrink the injection profile to maintain the same rising and falling slopes exhibited by the experimental profile. Figure 6 shows the injection profiles used for each fueling level.

Figure 7 shows the predicted cylinder pressure and heat release rate for each case. As the quantity of fuel participating in HCCI combustion was decreased from pure HCCI combustion, a decrease in peak cylinder pressure was observed. Decreasing the quantity of premixed fuel also resulted in a retardation of the first stage combustion phasing.

Figure 8 shows the emission and performance characteristics for each quantity of premixed fuel. The HCCI case shows the lowest NO_x, HC, and CO emissions; however, the pressure rise rate was excessive at ~25 bar/deg. It was unexpected that the

**Figure 6.** Injection profiles used for preliminary TSC concept investigation normalized by the peak value of the diesel case. The percentages shown in the figure are the fraction of total fuel premixed at IVC.**Figure 7.** Cylinder pressure and heat release rate for each case. The percentages shown are the fraction of total fuel premixed at IVC.

pure HCCI case would show lower HC and CO emissions than the diesel case, as HCCI combustion is generally viewed as having relatively high HC and CO levels due to low combustion temperatures. It is likely that the relatively low HC and CO emissions of the pure HCCI case are due to the fact that no injection was considered; thus no wall wetting was present. Furthermore, the injection timing for the diesel case was very late (SOI timing at TDC), thus resulting in the higher than expected HC and CO emissions of the diesel case.

As fuel is removed from the HCCI combustion event and introduced to the cylinder via a late injection, the combustion phasing shifts towards TDC, a decrease in peak pressure rise rate is observed, NO_x and CO

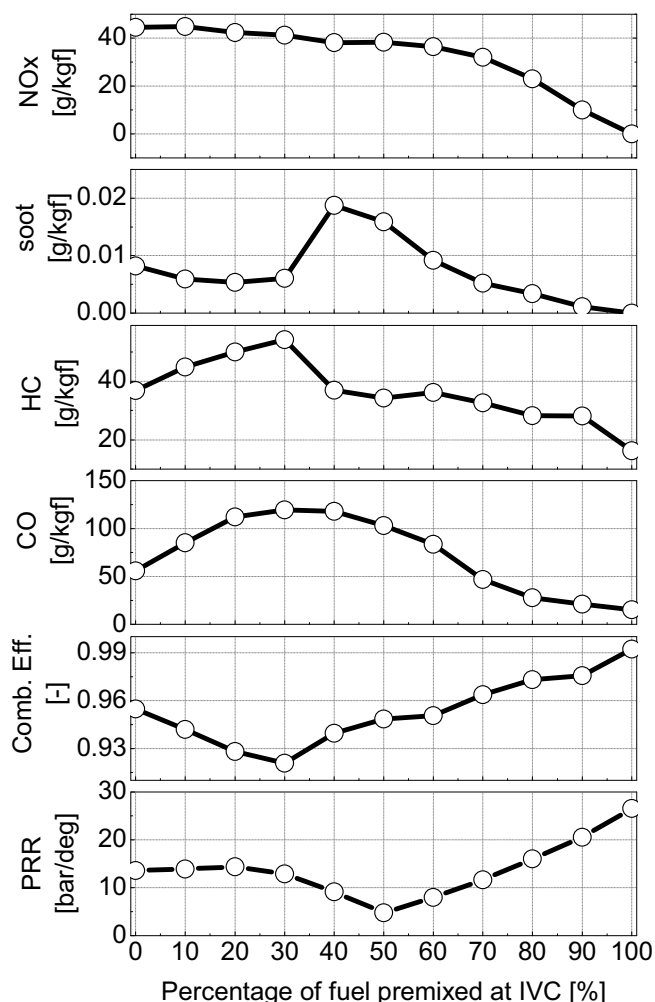


Figure 8. Effects of fraction of fuel premixed at IVC on NO_x, soot, HC, CO, combustion efficiency, and peak pressure rise rate.

increase dramatically, and HC increases slightly. As greater than 50% of the total fuel is removed from the HCCI event and placed in the late injection, combustion is delayed until after TDC, an increase in pressure rise rate is observed, NO_x remains almost constant, while HC and CO show an initial increase, then rapid decrease. The increase in pressure rise rate as the fraction of fuel participating in HCCI combustion is decreased beyond 50% is due to ignition delay of the late injection. When greater than 50% of the total fuel participates in HCCI combustion a cool flame heat release is observed followed by premixed heat release of the first stage fuel and a late injection diffusion burn near TDC, shown in Figure 7. As the fraction of fuel participating in HCCI combustion is decreased past 50%, very little cool flame heat release is observed and no premixed heat release is present. The ignition delay of the late injection increases as the fraction of fuel participating in combustion from the premixed fuel decreases. The increase in ignition delay allows significant time for mixing, resulting in rapid heat release and high pressure rise rates.

To gain an understanding of the combustion characteristics of cases with different quantities of premixed fuel,

temperature contours are presented for several times during the injection event, shown in Figure 9. Two cases are investigated, 20% premixed fuel and 70% premixed fuel. The heat release traces for the 20% premixed fuel case showed no high temperature heat release from the premixed fuel, resulting in a bulk gas temperature at the start of the late injection of only 950 K. The 70% premixed fuel case exhibited significant heat release from the premixed fuel resulting in bulk gas temperatures of 1560 K at the start of the late injection. The temperature contours of the 70% premixed fuel case show increased temperatures surrounding the spray plume almost immediately after fuel is injected. The fuel burns relatively slowly with a combustion duration of ~14 degrees. The spray images show spray-wall impingement occurs even with the elevated temperatures due to combustion from the premixed fuel. The liquid-phase fuel penetration correlation of Seibers [26] suggests the liquid length for this condition would be significantly shorter than the model predictions (around 12 mm rather than 20 mm). This may be due to an insufficient prediction of the droplet breakup at late injection conditions, thus resulting in an under prediction of droplet evaporation and extended liquid lengths. Spray model validation is ongoing.

The images of the 20% fuel case show that almost all of the fuel has been injected by the time heat is released from the late injection. The resulting combustion shows the characteristics of a premixed heat release with rapid combustion and high pressure rise rates. The combustion characteristics of the 20% premixed fuel case are very similar to those exhibited by the UNIBUS strategy of Hasegawa and Yanagihara [8].

The NO_x trends can be explained by examining the peak temperature histories of each case, shown in Figure 10. The maximum temperature for the first stage combustion in all cases remains well below 2000 K, therefore very little NO_x is formed during the first stage burn. The second stage combustion shows similar peak temperatures for all cases. The cases without premixed heat release (less than 50% premixed fuel) show similar temperature histories, resulting in similar NO_x levels. The cases with greater than 50% premixed fuel show that as the percentage of fuel injected late in the cycle increases, the temperature remains in the NO formation region for a longer period of time, resulting in higher NO_x levels.

The HC trend was investigated by comparing fuel mass fraction contours late in the cycle of the two cases previously discussed, 20% premixed fuel and 70% premixed fuel. Figure 11 shows images colored by fuel mass fraction after combustion. Both cases show significant unburnt fuel in the crevice region, however the 20% premixed fuel case also shows a large quantity of unburnt fuel on the piston top-land region near the wall. Because first stage combustion was not present in the 20% premixed fuel case, the fuel in the piston top land

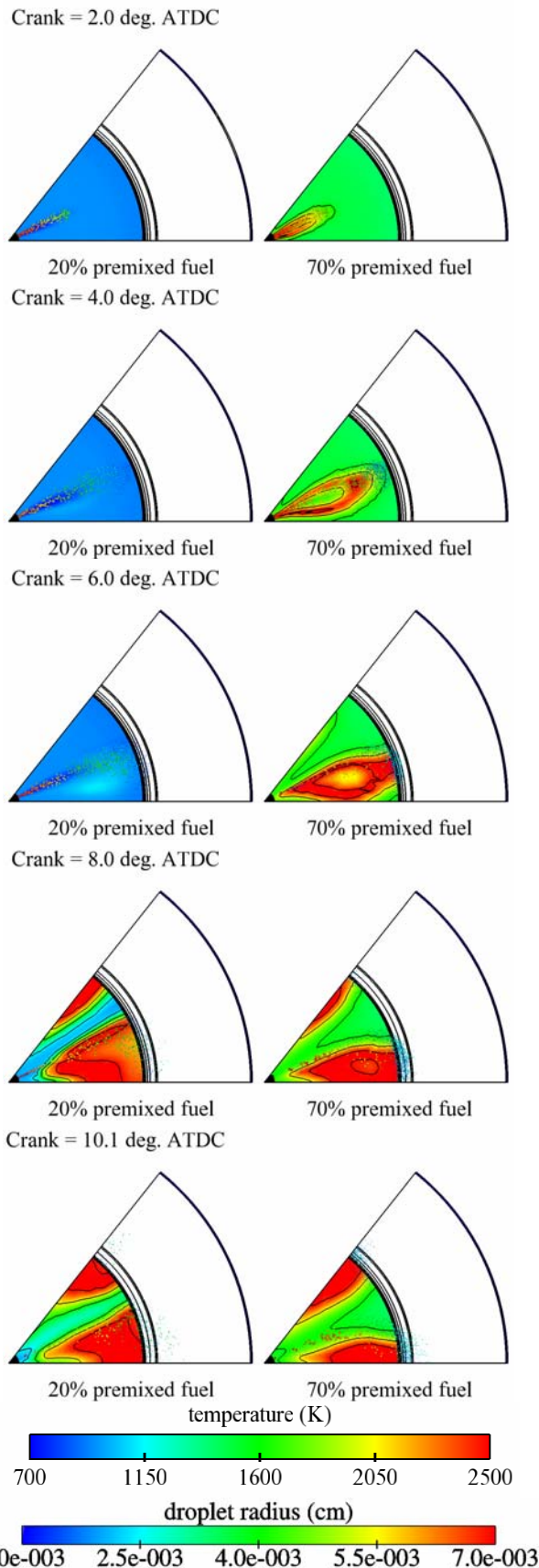


Figure 9. Temperature contours for two cases showing different combustion characteristics (20% and 70% premixed fuel). The cut-plane coincides with the spray axis. Droplets are sized and colored by drop radius.

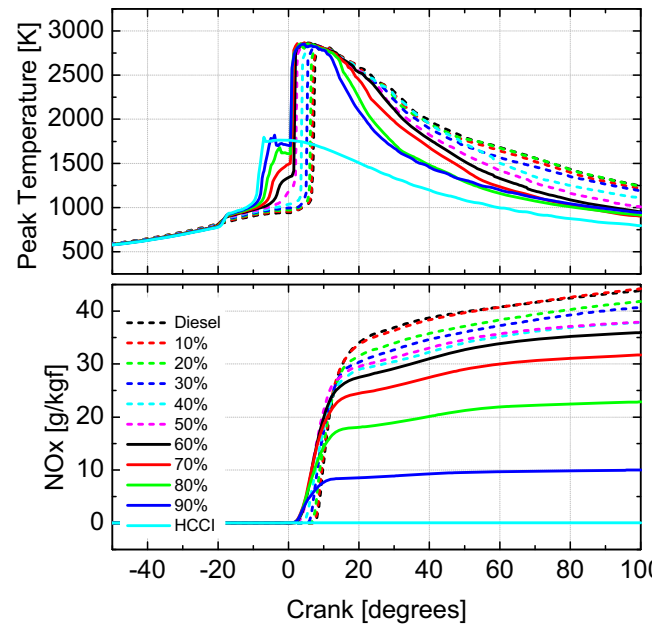


Figure 10. Peak in-cylinder temperature and NOx levels as a function of crank angle for each case. The percentages shown in the figure are the fraction of total fuel premixed at IVC

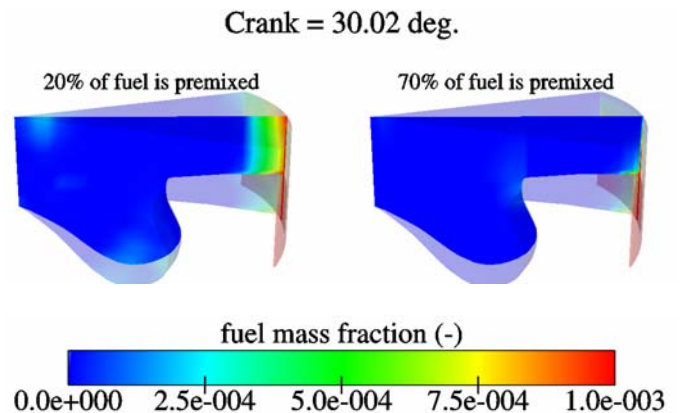


Figure 11. Fuel mass fraction contours at 30.2 degrees after TDC for two cases showing very different HC levels (20% and 70% of premixed fuel).

region was not consumed. Although the second stage combustion exhibited high temperatures in the bowl region, the temperatures near the cylinder wall remained low and the premixed fuel in this region was not oxidized.

The CO trend follows a similar pattern as that of the HC trend. As less fuel is premixed at IVC the equivalence ratio of the premixed fuel becomes excessively lean and combustion efficiency of the first stage deteriorates. When less than 50% of the total fuel is premixed, the first stage combustion is completely eliminated; however, a cool flame heat release still exists for these cases. The presence of a cool flame reaction