

Multi-Dimensional-Modeling-Based Development of a Novel 2-Zone Combustion Chamber Applied to Reactivity Controlled Compression Ignition Combustion

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ABSTRACT

A novel 2-zone combustion chamber concept (patent pending) was developed using multi-dimensional modeling. At minimum volume, an axial projection in the piston divides the volume into distinct zones joined by a communication channel. The projection provides a means to control the mixture formation and combustion phasing within each zone. The novel combustion system was applied to reactivity controlled compression ignition (RCCI) combustion in both light-duty and heavy-duty diesel engines.

Results from the study of an 8.8 bar BMEP, 2600 RPM operating condition are presented for the light-duty engine. The results from the heavy-duty engine are at an 18.1 bar BMEP, 1200 RPM operating condition.

The effect of several major design features were investigated including the volume split between the inner and outer combustion chamber volumes, the clearance (squish) height, and the top ring land (crevice) volume.

The results show significant improvements in the peak rate of pressure rise (ROPR), unburned hydrocarbon (UHC) emissions, and carbon monoxide (CO) emissions relative to open chamber RCCI combustion. Ultra-low soot and NOx emissions as well as a significant fuel consumption improvement, relative to conventional diesel combustion, were obtained with the novel 2-zone combustion chamber.

The novel 2-zone combustion system allows later, ignition controlling, diesel injection timings to be used while maintaining low UHC and CO emissions. Therefore control over combustion phasing and the peak ROPR are enhanced.

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INTRODUCTION

Conventional diesel combustion is ubiquitous in engine applications where low fuel consumption, durability, and / or sustained high load operation are of paramount importance. Conventional diesel combustion is well known for low UHC and CO emissions, as well as easily controlled combustion phasing and peak ROPR. However, due to the heterogeneous nature of the combustion process, relatively high levels of soot and NOx emissions result [1]. Moreover, strategies employed to reduce one of these emissions tend to exacerbate the other, resulting in the well-known soot vs. NOx tradeoff.

Under current legislated emissions rules, the levels of soot and NOx emissions resulting from conventional diesel combustion necessitate the use of after-treatment devices. Current emissions compliant diesel engines use a combination of EGR, high pressure fuel injection and aftertreatment devices such as SCR (Selective Catalytic Reduction). The modeling results show that the 2-zone combustion system

eliminates or reduces need for aftertreatment compared to diesel engines. The elimination of soot and NOx after-treatment devices could result in a significant cost savings.

Premixed compression ignition (PCI) combustion strategies have been developed to circumvent the soot vs. NOx trade-off [2, 3, 4]. The premixed nature of combustion mitigates soot formation allowing high levels of dilution (i.e., EGR) to reduce NOx. However, these strategies have proved difficult to implement in practical applications due to the loss of control over combustion phasing and peak ROPR.

More recently the RCCI combustion strategy has been developed to address the control issues and maintain the benefits of PCI [5, 6, 7, 8, 9, 10, 11, 12]. By using 2 fuels of differing reactivity the overall charge reactivity, as well as the reactivity stratification, can be tailored at various loads and speeds to properly phase combustion and enhance control over the peak ROPR. However, even with the

RCCI combustion, the peak ROPR has proven difficult to control at high loads and low speeds. RCCI combustion can also result in unacceptably high levels of UHC and CO emissions.

In this paper novel 2-zone combustion system (patent pending) is described, which has been developed using multi-dimensional modeling and which addresses the peak ROPR, UHC emissions, and CO emissions challenges while retaining the ultra-low soot and NOx emissions and reduced fuel consumption associated with RCCI combustion.

Figure 1 shows an example 2-zone piston geometry, along with a geometry typically seen in conventional diesel engines for comparison. The 2-zone chamber is characterized by a raised piston-divider section approximately half way between the center and the outer edge of the piston. When the piston is near the top-dead-center (TDC) position, the novel piston design divides the chamber into 2 zones connected by a passage defined by the clearance between the piston and cylinder head (squish height). Fuel injected during this time (shown as green cones) primarily mixes with the inner volume. The stratification from the late injection preferentially promotes ignition in the inner volume. Pressure differences between the inner and outer volumes generate relatively strong flows (depicted by the orange arrow) which serve to both ignite the outer volume and displace any fluid that has been cooled by proximity to the walls.

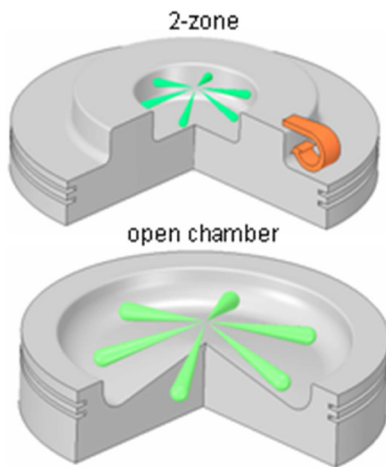


Figure 1. Example 2-zone piston geometry and conventional diesel geometry.

MULTI-DIMENSIONAL MODEL

Combustion simulations were performed using the KIVA-3V release 2 code [13] coupled with CHEMKIN II for detailed chemical kinetic calculations. Improvements have been made to many physical and chemistry models in the original KIVA-3V code [14, 15, 16, 17]. In this study, iso-octane was used as the gasoline surrogate, while n-heptane was chosen to represent diesel fuel chemistry. A reduced primary reference fuels (PRF) mechanism that contains 45 species and 142 reactions was used to simulate both gasoline (PRF100) and diesel fuel (PRF0) chemistry [18]. The physical properties of diesel fuel were modeled as tetradecane. The intake port injected gasoline was modeled as a homogeneous mixture at the beginning of the simulation, which started from intake valve closure (IVC) and ended at exhaust valve opening (EVO). A sector of the combustion chamber was modeled, including a single fuel spray.

Soot was predicted using a phenomenological model based on the approach developed by Hiroyasu [19]. Acetylene was used as an inception species in the soot model. The soot model was coupled to the chemistry solver through the addition of 13 reactions involving acetylene. NOx emissions were predicted using a reduced NO mechanism that includes 4 species and 12 reactions [20].

The spray model uses the Lagrangian-Drop and Eulerian-Fluid (LDEF) approach. Droplet breakup was modeled using the hybrid Kelvin Helmholtz (KH)-Rayleigh Taylor (RT) model described by Beale and Reitz [16]. The droplet collision model is based on O'Rourke's model, but a radius of influence method was used to determine the possible collision partners to further remove mesh dependency [15]. Interactions between droplets and the wall were considered via a wall film sub-model [21-22].

DESCRIPTION OF ENGINES AND OPERATING CONDITIONS

Table 1. Description of engines, operating conditions and baseline RCCI injection strategies.

	Light-Duty Engine	Heavy-Duty Engine
Bore (cm)	8.20	13.72
Stroke (cm)	9.04	17.15
Compression Ratio (-)	15.1	12.0
Number of Valves	4	4
IVC ($^{\circ}$ ATDC)	-132	-158
EVO ($^{\circ}$ ATDC)	112	113
Swirl Ratio at IVC (-)	2.2	0.6
BMEP (bar)	8.80	18.12
Engine Speed (rpm)	2600	1200
AFR (-)	31	15.1
EGR (%)	10	62.4
IVC temperature (K)	365	399
IVC pressure (bar)	1.86	4.21
Total Fuel (g)	0.0233	0.2447
DI Diesel Fuel %	12	12
Pre-mixed Gasoline %	88	88
1 st Diesel Injection %	100	66
2 nd Diesel Injection %	N/A	34
SOI 1 st Diesel Injection ($^{\circ}$ ATDC)	-56	-62
SOI 2 nd Diesel Injection ($^{\circ}$ ATDC)	N/A	-27
Number of Injector Holes (Direct Injection)	7	6
Hole Size (μ m)	141	114
Nozzle Included Spray Angle (deg.)	148	130
Diesel Injection Pressure (bar)	500	670

Table 1 contains a description of the light-duty and heavy-duty engines of interest. Also included is a description of the operating conditions, baseline RCCI fueling strategies, and diesel fuel injector

nozzle specifications. For the light-duty engine the gasoline was port injected and a single diesel injection event was used. For the heavy-duty engine the gasoline was port injected and 2 diesel injection events were used.

MODEL VALIDATION

The baseline pistons for both the LD [23] (see Figure 2) and HD (see Figure 4) engines were modified specifically for RCCI operation. In an effort to maximize combustion efficiency and reduce heat transfer, common diesel piston features such as a re-entrant bowl which add surface area were removed since that feature is used to promote mixing for conventional diesel combustion.

Light - Duty

The light-duty model validation was performed on data acquired from a GM 4-cylinder JTD 1.9L engine located at Oak Ridge National Lab. Engine data was collected over a range of speeds and loads relevant to the light-duty US drive cycle [24]. For the present work, the results of the model validation at one operating point are shown. The highest load operating point (8.80 bar BMEP 2600 rpm) in the drive cycle was used in the model validation and to develop the 2-zone concept.

A three dimensional computational grid with the crevice volume resolved, as shown in Figure 2, was used for the validation simulations. To reduce the computational burden, a 51.4° sector mesh (corresponding to a single nozzle hole of the seven hole injector) with periodic boundaries was used. This bowl geometry will be referred to as 'open' in the following analysis.

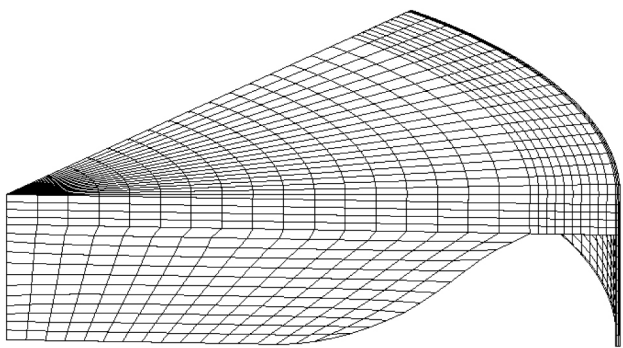


Figure 2. Baseline light-duty computational grid with crevice volume shown at -20° ATDC. The grid has 28,500 cells at bottom dead center (BDC).

Figure 3 shows the pressure and heat release for the model and test data. Overall, the phasing of pressure and heat release is well matched. The peak heat release magnitude is over-predicted for the model. Averaging of the experimental pressure data may be responsible for reducing the peak heat release. The phasing and location of peak pressure indicate that the average thermodynamic conditions are met during the simulations.

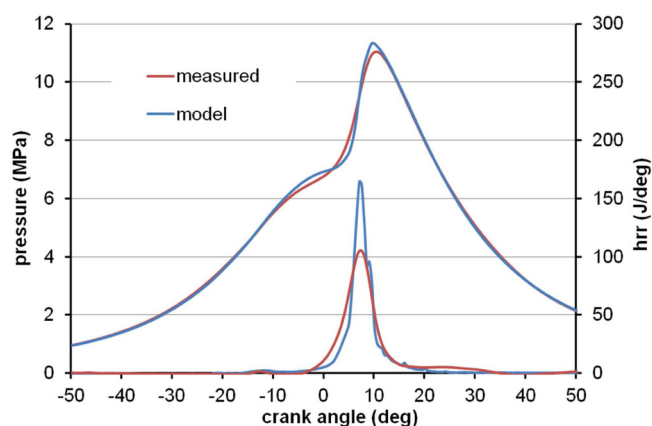


Figure 3. Baseline light-duty measured and modeled cylinder pressure and HRR vs. crank angle (ATDC).

The emissions results are shown in Table 2. The model under-predicts the NOx emissions. The CO and UHC are also under-predicted. The discrepancy between the modeled and measured results is attributed to variability of conditions inside the multi-cylinder engine that the model cannot account for. The port injected fuel and EGR are both introduced through the intake manifold. The manifold shares common passages between all cylinders which may further complicate the consistency of the initial fuel, air and EGR mixture. The coefficient of variance of peak pressure was 4.94 indicating the peak temperature can vary by 600K looking at +/- 3σ. Emissions predictions are temperature sensitive and may respond in a non-linear fashion. For the purposes of the model analysis that follows, the simulations will therefore only be used to provide a trend-wise comparison between cases.

Table 2. Baseline light-duty measured and modeled emissions.

	Measured	Modeled
NOx (ppm)	74	13
CO (ppm)	899	587
UHC (ppm)	2773	771

Heavy - Duty

Figure 4 shows the geometry used for the heavy duty model validation. It is a 60° axi-symmetric mesh and contains 36,000 cells at BDC. The piston was designed to demonstrate RCCI operation at high loads. For this reason, a low compression ratio of 12:1 was chosen to ensure flexibility in test calibrations. The grid did not include a crevice region at this time because a detail seen in the piston surface near the cylinder wall (see Figure 2 right) used up the crevice feature in the grid generation tool. For the HD engine, the model validation and initial comparisons to the 2-zone geometry were performed without crevice regions. A later section includes modeling results with crevice regions added to both the baseline (Figure 4) and 2-zone (Figure 11) grids.

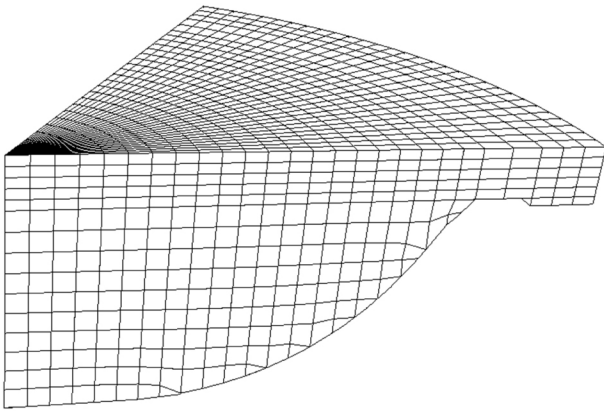


Figure 4. Baseline heavy-duty computational grid without crevice volume shown at TDC. The grid has 36,000 cells at BDC.

Figure 5 compares the measured and modeled cylinder pressure and heat release rate (HRR) vs. crank angle (ATDC) for the heavy-duty engine with an open chamber piston bowl geometry. Table 3 shows the measured and modeled peak ROPR and CO emissions. Near-zero soot and NOx emissions were measured experimentally and predicted by the model.

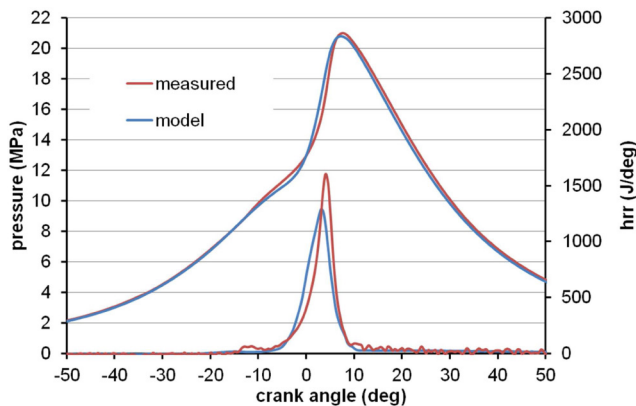


Figure 5. Baseline heavy-duty measured and modeled cylinder pressure and HRR vs. crank angle (ATDC).

Table 3. Baseline heavy-duty measured and modeled peak ROPR and CO emissions.

	measured	model
Peak ROPR (bar/deg.)	20.5	16.8
CO (g/kg-fuel)	31.9	56.2

RESULTS

Light - Duty

The 2-zone combustion system was examined with two different calibrations described as seen in Table 4. The open and 2-zone early calibration is exactly the same as that used for the validation. The second calibration, referred to as 2-zone late, uses less boost, lower injected fuel percentage, more EGR, and later start of injection (SOI). For the following discussion the open geometry refers to Figure 2.

The 2-zone geometry used for study in the light-duty engine is shown in Figure 6. The ratio of the outer to inner volume is 3 to 1. Further study of the effect of the volume split will be provided in the Heavy-Duty section. Considerations for the piston rings were necessary in determining the shape of the outer volume. Engine tests were conducted with this geometry and are available in another publication. Results with the 2-zone piston geometry are included in a companion publication [25].

First, global metrics including ROPR, fuel economy, NOx and CO will be compared. Following that is a detailed look at the spatial and temporal information related to 2-zone combustion system operation. Pre-mixed combustion strategies using auto-ignition can have high rates of pressure rise due to the volumetric nature of the combustion. The 2-zone piston bowl concept segregates the fuel-air mixture into two distinct zones connected by a communication channel. The mixture stoichiometry in each zone can then be tailored to control combustion phasing and rate. Control of the mixture preparation in each zone allows the inner volume to provide ignition. The outer volume can be prepared with a less reactive mixture by injecting little or no diesel into the outer volume.

Table 4. Operating parameters for 2-zone comparison.

Example	Open	2-zone early	2-zone late
BMEP (bar)	8.8	8.8	8.8
Engine Speed (rev/min)	2600	2600	2600
EGR rate (%)	10	10	28
IVC Temperature (°K)	365	365	365
IVC Pressure (bar)	1.85	1.85	1.75
Compression Ratio (-)	15.1	15.5	15.5
AFR (-)	31.0	31.0	23.0
Total Fuel (mg/cycle)	23.3	23.3	23.3
Pre-mixed Gasoline Mass Fraction (-)	0.88	0.88	0.95
Diesel Mass (mg/cycle)	2.8	2.8	1.1
Gasoline Mass (mg/cycle)	20.5	20.5	22.2
Diesel Injection Pressure (bar)	500	500	300
Diesel SOI1 (°ATDC)	-58	-58	-24
Diesel SOI2 (°ATDC)	n/a	n/a	n/a
Pulse 1 fraction (-)	100	100	100
Inner Volume (%)	100	25	25
Outer Volume (%)	n/a	75	75

Figure 7 shows the pressure and heat release for the three cases in Table 4. For the 2-zone cases the peak heat release rate is 50% and 75% lower for the early and late cases respectively. The differences in the ROPR were somewhat exaggerated because the model validation did not match the peak heat release well. The 2-zone late case has a maximum pressure 20% lower relative to the open bowl. For the