

Experiments and Modeling of Dual-Fuel HCCI and PCCI Combustion Using In-Cylinder Fuel Blending

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ABSTRACT

This study investigates the potential of controlling premixed charge compression ignition (PCCI and HCCI) combustion strategies by varying fuel reactivity. In-cylinder fuel blending using port fuel injection of gasoline and early cycle direct injection of diesel fuel was used for combustion phasing control at both high and low engine loads and was also effective to control the rate of pressure rise. The first part of the study used the KIVA-CHEMKIN code and a reduced primary reference fuel (PRF) mechanism to suggest optimized fuel blends and EGR combinations for HCCI operation at two engine loads (6 and 11 bar net IMEP). It was found that the minimum fuel consumption could not be achieved using either neat diesel fuel or neat gasoline alone, and that the optimal fuel reactivity required decreased with increasing load. For example, at 11 bar net IMEP, the optimum fuel blend and EGR rate for HCCI operation was found to be PRF 80 and 50%, respectively. Engine experiments using a dual-fuel PCCI strategy with port fuel injection of gasoline and early cycle multiple injections of diesel fuel with a conventional diesel injector (i.e., wide angle and large nozzle hole) were performed. The experimental results confirmed that an extension of the PCCI operating regime is possible when optimized fuel blends are used. At the 11 bar operating point, NO_x and soot were ~0.01 g/kW-hr and ~0.008 g/kW-hr, respectively. That is, US 2010 heavy duty emissions regulations are easily met without after-treatment while achieving 50% thermal efficiency.

INTRODUCTION

Rising fuel costs and a focus on reduction of greenhouse gases has driven the need for increased efficiency from the internal combustion engine. This need for increased efficiency has placed the diesel engine in the spotlight. Furthermore, current and future legislation place stringent standards on the exhaust emissions. These demands require development of advanced engine technologies, which can simultaneously yield high efficiency and low emissions.

Many strategies have been investigated to meet the future requirements of clean, efficient diesel engines. Most of the current strategies can be lumped into the category of low temperature premixed combustion. Lower combustion temperatures result in NO_x reduction due to the high activation energy of NO formation reactions [1]. In addition, utilizing long ignition delay times allows adequate time for mixing prior to the start of combustion; thus, rich regions are reduced and soot formation is inhibited. Many researchers have shown Homogeneous Charge Compression Ignition (HCCI) and Premixed Charge Compression Ignition (PCCI) concepts to be promising techniques for simultaneous NO_x and soot reduction [2-5]. Sun [6] has shown the PCCI, HCCI, and traditional diesel operating regimes on the equivalence ratio-temperature diagram, as shown in Figure 1. This diagram was originally presented by Kamimoto [7] and has been extensively discussed by Pickett et al. [8], Akihama et al. [9], and others.

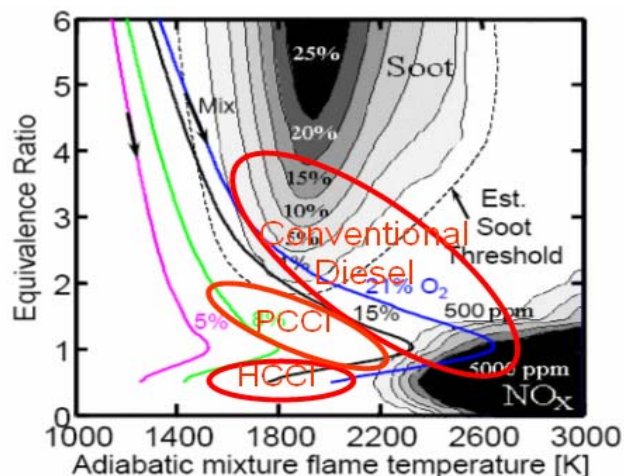


Figure 1. PCCI, HCCI, and conventional diesel operating regimes shown in T- Φ space [6].

Due to the existing fuel infrastructure, most HCCI and PCCI research has been conducted using either strictly gasoline or diesel fuel. However, in their neat forms, each fuel has specific advantages and shortcomings for premixed compression ignition (PCI) 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., [10, 11]). Conversely, diesel fuel has superior auto-ignition qualities; however, this can result in difficulty controlling the combustion phasing as engine load is increased. Therefore, when neat diesel fuel is used in a PCI strategy, high levels of exhaust gas recirculation (EGR) are required to phase combustion appropriately. Opat et al. [4] showed high efficiency, clean PCCI combustion at 5.5 bar IMEP using diesel fuel and ~67% EGR. However, high levels of EGR restrict high load operation due to reduced air flow. Furthermore, combustion phasing control during transient operation may be difficult when only EGR is used to control combustion phasing [12].

Recent experiments performed by Bessonette et al. [13] 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.

Inagaki et al. [12] investigated dual-fuel PCI operation as means for reducing the EGR requirements of PCI strategies. Using premixed iso-octane and direct

injection diesel fuel, they were able to operate in PCI mode at 12 bar IMEP. Furthermore, they showed that stratification of fuel reactivity (rather than only equivalence ratio) resulted in reduced rates of heat release and reasonable combustion noise.

Based on the work of Bessonette et al. [13] and Inagaki et al. [12], 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 gasoline and early cycle direct injection of diesel fuel.

SCOPE AND OBJECTIVES

The objective of this study is to explore fuel blending as a means for extending the PCCI operating regime. In this study gasoline and diesel fuel blends are used to address several issues associated with premixed charge compression ignition (PCCI and HCCI) combustion strategies, viz.: lack of combustion phasing control at high engine loads and excessive rates of pressure rise. In-cylinder fuel blending using port fuel injection of gasoline and early cycle direct injection of diesel fuel is proposed as the fuel delivery and blending strategy. By using in-cylinder fuel blending, the fuel reactivity can be adjusted on a cycle-to-cycle basis by changing the injected quantities of gasoline and diesel fuel to optimally accommodate engine load and speed changes. Furthermore, reactivity stratification may be beneficial in reducing combustion noise.

EXPERIMENTAL SETUP

ENGINE

A heavy-duty 2.44 l Caterpillar 3401 Single Cylinder Oil Test Engine (SCOTE) was used for all the engine tests. The specific engine geometry and configuration are given in Table 1 and the lab setup is given in Figure 2.

Table 1. Test engine geometry

Base engine type.....	Caterpillar SCOTE
Bore x stroke	13.72 x 16.51cm
Connecting Rod Length.....	21.16 cm
Squish height.....	0.157 cm
Displacement.....	2.44 L
Geometric compression ratio.....	16.1:1
Effective compression ratio.....	9.1:1
Swirl ratio.....	0.7
Bowl type	“Mexican Hat”
Number of valves	4
Intake valve opening	-335° ATDC Firing
Intake valve closing	-85° ATDC Firing
Exhaust valve opening	130° ATDC Firing
Exhaust valve closing.....	-355° ATDC Firing

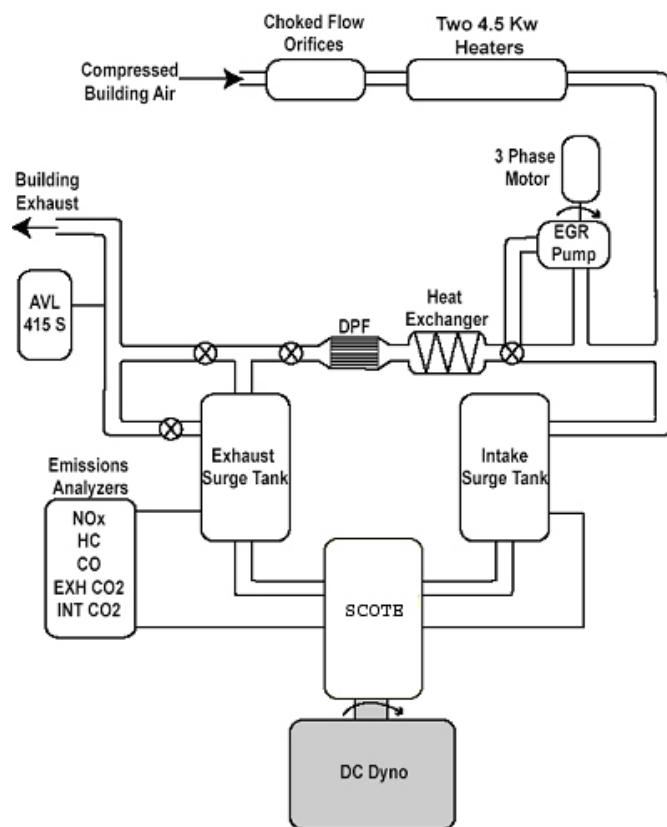


Figure 2. Diagram of the engine lab setup

INJECTION SYSTEM

Preliminary dual-fuel HCCI engine experiments were performed using port fuel injection of gasoline and direct injection near BDC of diesel fuel using an automotive Gasoline Direct Injection (GDI) type injector[†]. The specifications for the port fuel injector and GDI injector are given in Table 2 and Table 3, respectively. Dual-fuel PCCI operation was also explored using the port fuel injector of Table 2 for gasoline delivery and a conventional type (i.e., wide angle, large nozzle hole) high pressure common rail diesel injector for diesel fuel delivery. The specifications for the common rail injector are given in Table 4.

Table 2. Port fuel injector specifications

Steady flow rate @ 3 bar	12.5 cc/sec
Included spray angle	15°
Fuel pressure	5.17 bar

Table 3. GDI injector specifications

Number of holes	6
Steady flow rate @ 100 bar	12.8 cc/sec
Hole diameter	165 μ m
Included spray angle	60°

Table 4. Common rail injector specifications

Number of holes	6
Steady flow rate @100 bar	33.3 cc/sec
Hole diameter	250 μ m
Included spray angle	145°
Injection pressure	600 and 800 bar

DATA ACQUISITION AND LABORATORY HARDWARE

Cylinder pressure was measured with a Kistler model 6043 Asp water-cooled pressure transducer in conjunction with a Kistler model 510 charge amplifier. Acquired cylinder pressure traces were averaged for 500 cycles to smooth pressure data due to the ringing experienced from PCI combustion. Intake air flow was measured using choked flow orifices. To obtain choked flow for a variety of engine operating conditions, combinations of 6 different sized orifices were used to gain the desired intake air flow rate. Intake air was heated with two immersion style heaters and PID control to $\pm 1^\circ\text{C}$. Both the intake and exhaust system surge tank pressures were equipped with PID control to ± 0.7 kPa. PM measurements were performed with an AVL model 415s smoke meter. PM measurements of filter smoke number (FSN), mass per volume (mg/m^3) and specific emissions (g/kWh) were related with the factory AVL calibration and averaged between 5 samples of a 2 l

[†] Sun et al. [15] showed that for very early injection timings (near BDC), liquid impingement on the cylinder liner was significantly reduced when a low-pressure, narrow angle, GDI-type injector was used rather than a conventional, high-pressure, wide-angle diesel injector.

CAMSHAFT

To lower peak cylinder pressures and aid in combustion phasing control, different methods of modifying intake valve closing timing were investigated by Nevin [14]. Nevin examined 4 different custom camshafts with intake valve closing (IVC) timings ranging from 143 BTDC (stock) to 85 BTDC in order to lower the effective compression ratio, see Figure 3. The IVC85 cam was found to lower the peak cylinder pressures 10 bar from stock [14] and was used for all tests in this paper.

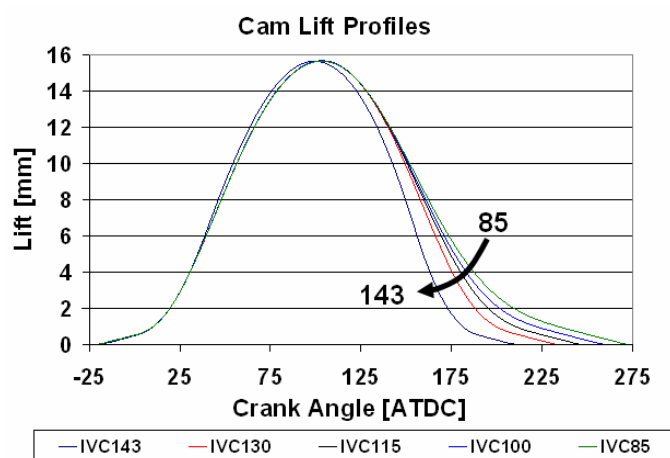


Figure 3. Intake valve lift profiles for custom camshafts

volume each with paper saving mode off. All gaseous emissions measurements were performed with a 5 gas emissions bench. The details of the gaseous emissions measurements are given in Table 5. The EGR rate was determined through the ratio of intake CO₂ to exhaust CO₂ levels. Gaseous emissions were averaged for 30 seconds after attaining steady-state for several minutes.

Table 5. Details of the gaseous emission measurement instruments

Species	Manufacturer /Model	Method
NO/NO _x	California Analytic Instruments 400S-HCLD	Heated-Chemiluminescence Detector
CO	California Analytic Instruments 3300A	Non-dispersive Infrared Light Absorption
Intake CO ₂	California Analytic Instruments 100	Non-dispersive Infrared Light Absorption
Exhaust CO ₂	Siemens 5E-2R	Non Dispersive Infrared Light Absorption
UHC	Siemens FIDAMAT 5E-im	Heated Flame Ionization Detector

EGR SYSTEM

The EGR system consisted of an electrically driven supercharger and a diesel particulate filter (DPF), to prevent fouling of the EGR cooler and supercharger. The EGR supercharger was implemented as a pump to maintain constant EGR levels with constant surge tank pressures as the DPF fills. Conversely, the use of the supercharger in this manner allows experimental simulations with more than practical turbocharger efficiency levels, if the pressure difference between the intake and exhaust surge tanks were small. However, effort was taken to avoid such conditions.

FUEL PROPERTIES

Commercially available 91 pump octane number (PON[†]) gasoline and ULSD were used for all tests. Table 6 and Table 7 show an independent lab analysis of the fuel properties.

COMPUTATIONAL MODEL

Computations are performed using the KIVA-3v release 2 code [16] with improvements to many physical and chemistry models developed at the ERC [17-19]. The KIVA-3v code is coupled with the CHEMKIN II solver for detailed chemistry calculations. Gasoline and diesel fuel chemistry is represented by that of iso-octane and n-heptane, respectively. A 45 species and 142 reaction mechanism for primary reference fuels (PRF) [20] is

[†] PON=(RON+MON)/2. PON is also referred to as the antiknock index.

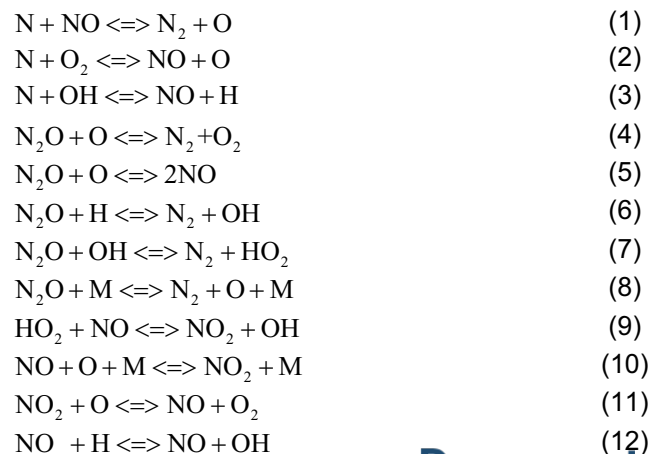
Table 6. Gasoline fuel properties

Distillation Curve	ASTM D86
Initial Boiling Point.....	38.9 °C
Temperature 10% evaporated.....	69.4 °C
Temperature 50% evaporated.....	105.0 °C
Temperature 90% evaporated.....	160.6 °C
Final Boiling Point	215.6 °C
Lower Heating Value	43.2 MJ/kg
MON.....	87.8
RON	95.6
(R+M)/2.....	91.6
Ethanol	0 %
H/C ratio	1.88
Density	756 kg/m ³

Table 7. Diesel fuel properties

Viscosity (@ 40 °C)	2.71 cSt
Surface Tension (@ 25 °C)	30.0 dyne/cm
Lower Heating Value	42.526 MJ/kg
Cetane Number.....	46.1
H/C ratio	1.74
Density	856 kg/m ³

used to simulate gasoline and diesel fuel chemistry. Many studies (e.g., Ra et al. [21]) have shown that the combustion characteristics of gasoline and diesel are represented well by iso-octane (i.e., PRF 100) and n-heptane (i.e., PRF 0), respectively. The physical properties (for spray and mixing processes) of diesel fuel are represented by tetradecane. This modeling approach has been shown to yield acceptable results in numerous studies (e.g., Kong et al. [22]). Soot is predicted using a phenomenological soot model [22] based on the approach of Hiroyasu [23]. The soot model used in the present study uses 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 are 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 [24]. The reduced NO mechanism described by Sun [6] is shown below:



Because detailed chemistry calculations are often time consuming, the Adaptive Multi-grid Chemistry (AMC) model of Shi et al. [25] is employed. The AMC model reduces the number of cells that need to be computed by the chemistry solver by grouping cells with similar gas properties for chemistry calculations and remapping the results to the original mesh. Previous investigations by Shi et al. [26] showed computational times were reduced by more than a factor of three while maintaining an accurate prediction of the emissions results.

The spray model employed in this study uses the Lagrangian-Drop and Eulerian-Fluid (LDEF) approach. Because a detailed chemistry model is used, it is desirable to use a relatively coarse computational mesh; however, severe grid size dependency has been observed in LDEF spray models. This problem is most severe in the near nozzle region where the droplets are very close together and occupy only a small portion of the Eulerian mesh. Abraham [27] showed that accurate modeling of the near nozzle region required grid resolution on the order of the orifice diameter. However, it is not feasible from a computational time standpoint to solve engine problems on such a fine mesh. Furthermore, a fundamental assumption of the LDEF approach is that the volume fraction of droplets in each cell is small, that is, the void fraction is near one. Thus, if the mesh size is overly refined (i.e., mesh size of the order of the droplet size) this assumption may be violated. In order to reduce the grid size dependency of the LDEF spray model and allow accurate spray simulation on a relatively coarse grid, the Gasjet model of Abani et al. [18] is employed to model the relative velocity between the droplets and gas phase in the near nozzle region. Their approach assumes that the relative velocity between a droplet and the gas phase is equal to that between the droplet and a turbulent gas-jet with the same mass and momentum of that of the injected fuel. This approach imposes an axial component for the gas phase velocity as a function of distance from the nozzle, which is used in the droplet acceleration equation given by:

$$\frac{dU}{dt} = \frac{3}{8} C_D \frac{\rho_g}{\rho_l r_d} |U - V_{gas}| (U - V_{gas}) \quad (13)$$

where U is the droplet velocity vector, C_D is the droplet drag coefficient which is a function of Reynolds number, ρ_g and ρ_l are the gas and liquid phase densities respectively, r_d is the droplet radius, and V_{gas} is the gas phase velocity vector given as $V_{gas} = (V_x, V_y, V_z)$ where V_y and V_z are the perpendicular to the spray axis and obtained from the Eulerian gas phase solution and V_x , the axial component of the gas phase velocity, is found from gas-jet theory [28] as:

$$V_x = U_{inj} \min \left[1, \frac{3d_{noz} \sqrt{\frac{\rho_l}{\rho_g}}}{K_{entr} x} \left(1 + \frac{12r^2}{K_{entr}^2 x^2} \right)^{-2} \right] \quad (14)$$

where U_{inj} is the injection velocity, d_{noz} is the nozzle diameter, K_{entr} is a model constant taken to be 0.7 as suggested by Abani et al. [18], x is the position downstream of the nozzle on the spray axis, and r is the radial position.

Droplet breakup is modeled using the hybrid Kelvin Helmholtz (KH) – Rayleigh Taylor (RT) model described by Beale and Reitz [29]. 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 reduce mesh dependency [18]. In addition, the collision model was expanded by Munnannur [30] to include a more comprehensive range of collision outcomes. The current implementation of the droplet collision model considers bounce, coalescence, and fragmenting and non-fragmenting separations. Droplet interactions with the wall are considered through a wall film submodel [31, 32], which includes the effects associated with splash, film spreading, and motion due to inertia.

A three dimensional computational grid with the crevice volume resolved was used, as shown in Figure 4. To reduce computational burden, a 60 degree sector mesh (corresponding to a single nozzle hole of the six hole injector of this study) with periodic boundaries was used for spray simulations and a 0.5 degree sector with periodic boundaries was used for HCCI simulations. The crevice above the top piston ring (between the piston and liner) is resolved and the region behind the ring is represented as an additional volume attached to the top ring crevice. Furthermore, the volumes associated with the head gasket, valve pockets, and pressure transducer crevices are added to the volume attached to the top ring crevice in order to give the correct compression ratio.

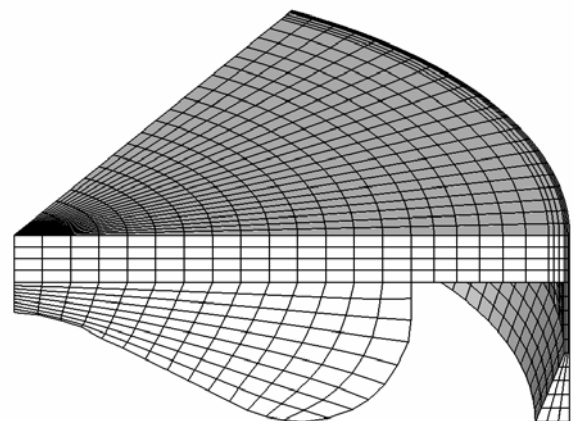


Figure 4. Computational grid with crevice volume shown at 16 °BTDC. The grid has 8500 cells at BDC.