

An Experimental Investigation of Fuel Reactivity Controlled PCCI Combustion in a Heavy-Duty Engine

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ABSTRACT

This study investigates the potential of controlling premixed charge compression ignition (PCCI) 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 a medium engine load of 9 bar net IMEP and was also found to be effective to prevent excessive rates of pressure rise. Parameters used in the experiments were guided from the KIVA-CHEMKIN code with a reduced primary reference fuel (PRF) mechanism including injection timings, fuel percentages, and intake valve closing (IVC) timings for dual-fuel PCCI combustion. The engine experiments were conducted with a conventional common rail injector (i.e., wide angle and large nozzle hole) and demonstrated control and versatility of dual-fuel PCCI combustion with the proper fuel blend, SOI and IVC timings. For example, at the 9 bar operating point, NO_x and soot were 0.012 g/kW-hr and 0.008 g/kW-hr, respectively. That is, US EPA 2010 heavy-duty NO_x and PM emissions regulations are easily met without after-treatment, while achieving 53% net indicated thermal efficiency.

Many strategies have been investigated to meet the future requirements of clean, efficient diesel engines. Most of the current strategies fall 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 a long ignition delay 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 [2,3,4,5]. Neely, et al, [6] represented the PCCI, HCCI, and traditional diesel operating regimes on the local equivalence ratio-temperature diagram, see [Figure 1](#). This diagram was originally presented by Kamimoto [7] and has been extensively discussed by Pickett et al. [8] and Akihama et al. [9]

INTRODUCTION

Rising fuel costs and a focus on reduction of greenhouse gases has driven a need for increased efficiency from the internal combustion engine. This need for increased efficiency has placed the diesel engine in the spotlight due to its higher efficiency compared to other engines. Furthermore, current and future legislation place stringent standards on the exhaust emissions. These demands require the development of advanced engine technology, which can simultaneously yield high efficiency and low emissions. Thus, it is important to control pollutant emissions from diesel engines.

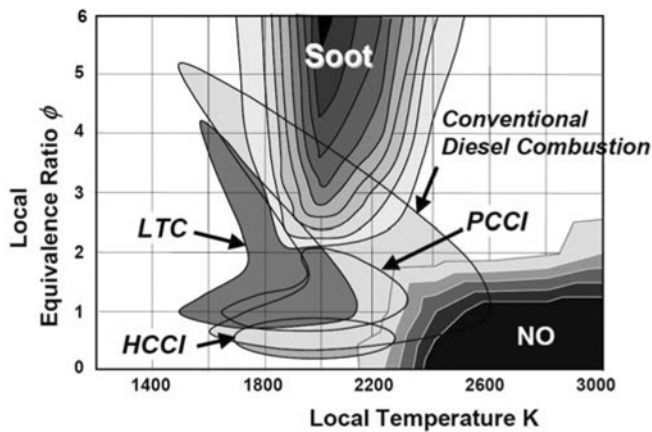


Figure 1. PCCI, HCCI, and conventional diesel operating regimes shown in Φ - T space [6].

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 PCCI 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 PCCI 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 the 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] suggested that the best fuel for HCCI operation may have autoignition qualities between those of diesel fuel and gasoline. Using a compression ratio of 12:1 and a fuel with a derived cetane number (DCN) 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 PCCI operation as means for reducing the EGR requirements of PCCI strategies.

Using premixed iso-octane and direct injection diesel fuel, they were able to operate in PCCI 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 with rapid in-cylinder fuel blending.

The objective of this study was 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 PCCI combustion strategies, i.e.: 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 control may be beneficial in reducing combustion noise.

Previous work by the authors [14] numerically and experimentally investigated PCCI dual-fuel combustion at both low and mid load conditions and achieved emissions levels below EPA 2010 heavy-duty limits in-cylinder, with out the need for aftertreatment, while maintaining low PRR and thermal efficiencies above 50%. The present study further explores this combustion strategy by varying the operating load range, SOI and IVC timings, and explores the effect of engine compression ratio.

EXPERIMENTAL SETUP

A heavy-duty 2.44 L Caterpillar 3401 Single Cylinder Oil Test Engine (SCOTE) was used for all the engine tests. The engine geometry is summarized in [Table 1](#) and the lab setup is shown in [Figure 2](#).

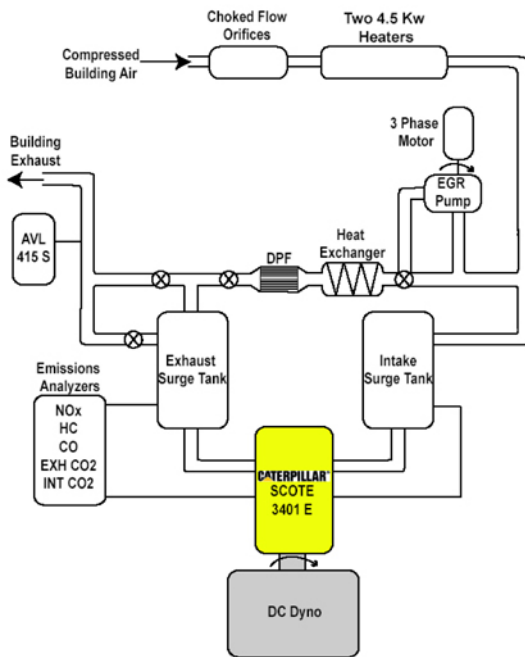


Figure 2. Diagram of the engine lab setup

Table 1. Caterpillar 3401E SCOTE engine geometry

Displacement (L)	2.44
Geometric Compression Ratio (-)	16.1:1
Effective Compression Ratio (-)	15.1-9.1:1
Squish Height (mm)	1.97
Bowl Volume (mL)	110.8
Connecting Rod Length (mm)	261.6
Bore x Stroke (mm)	137.2 x 165.1
Piston	Standard SCOTE
Valvetrain	EVC = -355 deg (°ATDC) compression IVC = -143 to -85 deg (°ATDC) EVO = 130 deg (°ATDC) compression IVO = 335 deg (°ATDC) compression
Swirl Ratio	Stock = 0.7

To lower peak cylinder pressures and aid in combustion phasing control, different methods of modifying intake valve closing (IVC) timing were investigated by Nevin [14], who used four different custom manufactured camshafts with IVC timings ranging from -143° ATDC (stock) to -85° ATDC in order to lower the effective compression ratio. The intake valve lift profiles are shown in Figure 3.

Initial CFD modeling results suggested the IVC timing of -85° ATDC would be optimal, due to the resulting lower TDC temperatures and pressures. However, in the present study, IVC timings closer to those utilized in the production 3406 engine were investigated by using three camshafts with IVC timings of -85 , -115 and -143° ATDC.

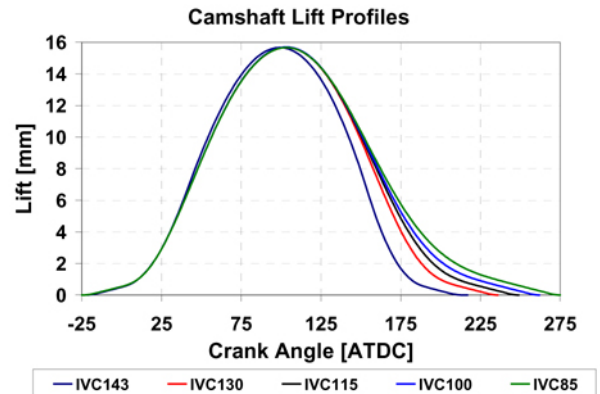


Figure 3. Intake valve lift profiles for custom camshafts

The dual-fuel PCCI engine experiments were performed using port fuel injection of gasoline and early direct injection of diesel fuel with a conventional (i.e., wide angle, large nozzle hole) Bosch high-pressure, common-rail injector. The specifications for the port fuel injector and common rail injector are given in Table 2 and Table 3, respectively.

Table 2. Port fuel injector specifications

Injection Pressure (MPa)	0.5
Included Spray Angle	15°
Number of Holes	3
Steady Flowrate (cc/min)	750

Table 3. Common rail injector specifications

Injection Pressure (MPa)	150
Included Spray Angle	145°
Number of Holes	6
Hole Diameter (μm)	250
Steady Flowrate (cc/30 sec) at 100 bar	1000

Cylinder pressure was measured with a Kistler model 6067C1 water-cooled pressure transducer in conjunction with a Kistler model 510 charge amplifier. Acquired cylinder pressure traces were averaged for 500 cycles to aid in smoothing pressure data. The intake air flow rate was measured using choked flow orifices. To obtain a choked flow condition 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 used PID control the temperature to within $\pm 1^{\circ}\text{C}$. Both the intake and exhaust system pressures were equipped with PID control to maintain the pressures ± 0.7 kPa. PM measurements were performed with an AVL model 415s smoke meter. PM measurements of filter smoke number (FSN), concentration (mg/m^3) and specific emissions (g/kWh) were related with the factory AVL calibration and averaged between 5 samples of a 2-L

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

The EGR system consisted of an electrically driven supercharger and a diesel particulate filter (DPF), to prevent potential 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 more repeatable and stable EGR rates.

Commercially available 91 pump octane number (PON[†]) gasoline and ultra low sulfur diesel (ULSD) were used for all tests. Table 4 and Table 5 show an independent lab analysis of the fuel properties.

Table 4. Diesel fuel properties

Specific Gravity (@ 15.5 °C) (-)	0.856
Viscosity (@ 40 °C) (cSt)	2.71
Surface Tension (@ 25 °C)	30
Lower Heating Value (MJ/kg)	42.526
Cetane Number	46.1
H/C ratio	1.74

Table 5. Gasoline fuel properties

Distillation Curve	ASTM
Initial Boiling Point (°C)	38.89
Temperature 10% evaporated (°C)	69.4
Temperature 50% evaporated (°C)	105
Temperature 90% evaporated (°C)	160.56
Final Boiling Point (°C)	215.56
Lower Heating Value (MJ/kg)	43.22
MON	87.8
RON	95.6
(RON+MON)/2	91.6
Ethanol (%)	0
H/C ratio	1.88
Specific Gravity (@ 15.6 °C) (-)	0.737
Sulfur (ASTM D5453) (PPM)	4.6

COMPUTATIONAL MODEL

Computations were performed to guide the selection of experimental operating parameters using the KIVA-3v release 2 code [16] with improvements to many physical and chemistry models developed at the ERC [17,18,19]. The KIVA-3v code is coupled with the CHEMKIN II solver for detailed chemistry calculations. A 39 species and 131 reaction mechanism for n-heptane [20] was used to simulate diesel fuel chemistry. Soot is predicted using a phenomenological soot model [21] based on the approach of Hiroyasu [22]. 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 [23].

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 the 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 [24] 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 equal to 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] was employed to model the relative velocity between the droplets and gas phase in the near-nozzle region. Their approach assumes that the relative velocity of 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 position from the nozzle, which is used in the droplet acceleration equation given by:

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

[†]PON=(RON+MON)/2, also referred to as the anti knock index

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 [25] 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 was modeled using the hybrid Kelvin Helmholtz (KH) - Rayleigh Taylor (RT) model described by Beale and Reitz [26]. The droplet collision model is based on O'Rourke's model; however, a radius of influence method was used to determine the possible collision partners to further reduce mesh dependency [18]. In addition, the collision model was expanded by Munnannur [27] 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 [28, 29], 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. The crevice above the top piston ring (between the piston and liner) was resolved and the ring-pack region behind the ring was 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 were added to the volume attached to the top ring crevice in order to give the correct compression ratio.

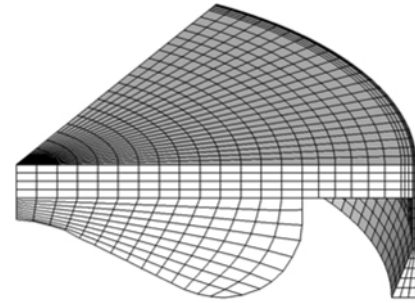


Figure 4. Computational grid with crevice volume shown at 16 °BTDC. The grid has 8500 cells at BDC.

RESULTS AND DISCUSSION

EFFECT OF FIRST MAIN INJECTION (SOI1) TIMING

The engine experiments were conducted at 9 bar net IMEP and 1300 rev/min and the operating conditions for the first main injection timing (SOI1) sweep are given in Table 6. Note that this case had 73% (by mass of the total fuel) port injected gasoline, with the remaining 27% as diesel fuel. The diesel fuel was injected using two injections with 62% of the diesel fuel quantity in the first injection. Figure 5 shows the experimental and modeled cylinder pressure and rate of heat release data for the SOI1 timing sweep. Figure 6 shows the corresponding emissions and performance characteristics for both the modeling and engine experiments. As the SOI1 timing is advanced, it is seen that combustion phasing is retarded, NOx and peak pressure rise rates are reduced, and an increase in CO is observed. It is interesting to note that HC emissions remain relatively flat. This suggests that the amount of spray liner impingement is not increasing with an advance in SOI1 timing. The authors previously investigated the source of HC in dual-fuel operation [14] and found that unreacted gasoline in the piston-liner crevice region accounts for most of the HC emissions at EVO.

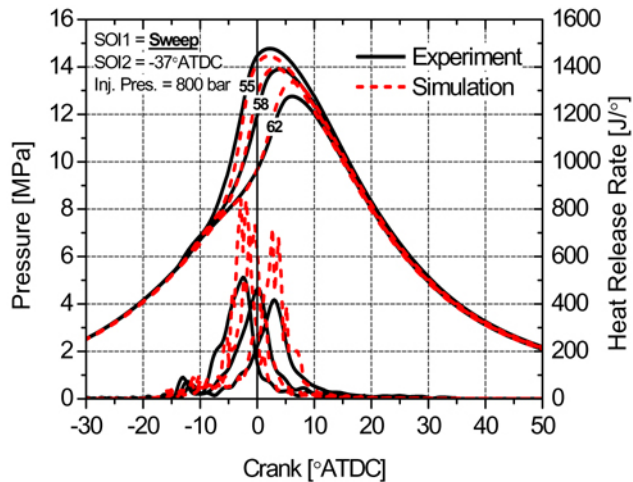


Figure 5. Measured and computed cylinder pressure and rate of heat release over a SOI1 timing sweep from -62 to -55 °ATDC.

Table 6. Operating conditions for the SOI1 timing sweep.

Nominal net IMEP (bar)	9			
Engine speed (rev/min)	1300			
IVC timing (°ATDC)	-85			
EGR rate (%)	43			
Equivalence ratio (-)	0.5			
Intake temperature (°C)	32			
Intake pressure (bar)	2			
Total fuel (mg/cycle)	97			
Percent gasoline by mass (%)	73			
Mass of diesel fuel (mg/cycle)	26.2			
Mass of gasoline (mg/cycle)	70.8			
Diesel injection pressure (MPa)	80			
Diesel SOI1 (°ATDC)	-55	-58	-60	-62
Diesel SOI2 (°ATDC)	-37			
Fract. of diesel fuel in pulse 1 (-)	0.62			
Diesel injection duration 1 (°CA)	5.47			
Diesel injection duration 2 (°CA)	3.12			

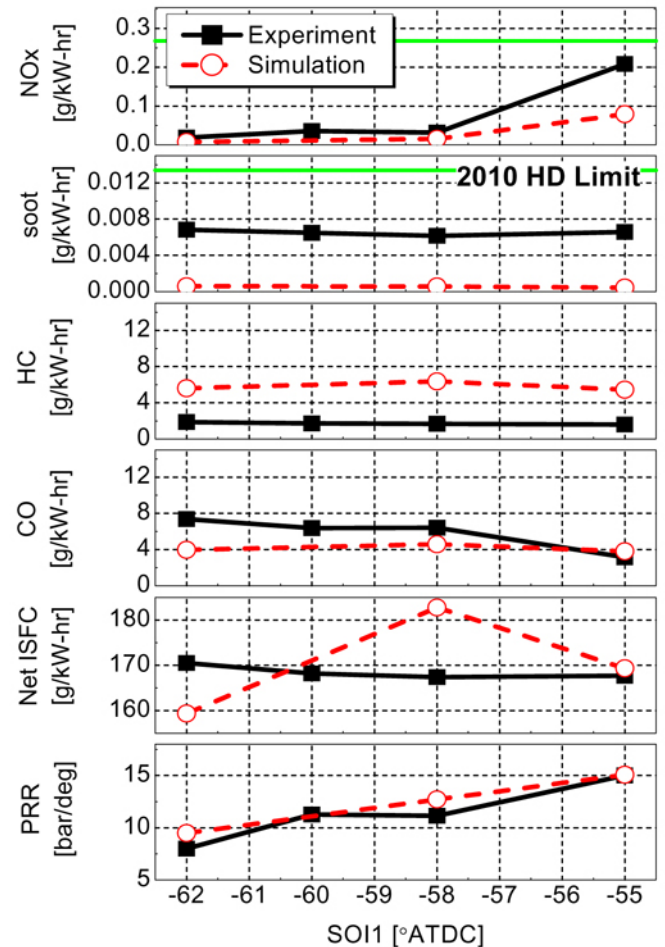


Figure 6. Measured and computed emissions and performance as a function of SOI1 timing.

Comparisons of the predicted and measured emissions show that the models are able to predict NO_x, CO, and peak pressure rise rate reasonably well. However, a significant under prediction of soot emissions is observed. It is thought that inhomogeneities at IVC, which are not modeled (recall that a homogeneous mixture of gasoline, air, and EGR was assumed at IVC), may contribute to differences in the predicted and measured soot levels. Additionally, soot formed from lube oil mist (i.e., lube oil entering the combustion chamber past the piston rings) is not modeled in the present study and may contribute to the observed under prediction of soot emissions. It likely that the soot model could have been tuned to yield acceptable agreement; however, since soot is not the focus of this study and measured soot levels were near zero, however this was not pursued. Furthermore, HC is over predicted. The over prediction of HC is likely due to the simplifications made to the crevice geometry. That is, in order to keep the squish height at the measured value, additional volume was added to the top piston ring crevice to account for the volume of the valve recesses, head gasket crevice, and pressure transducer