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Emissions from premixed charge compression ignition (PCCI) combustion and affect on emission control devices^{*}

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ABSTRACT

A light-duty diesel engine has been operated in advanced combustion modes known generally as premixed charge compression ignition (PCCI). The emissions have been characterized for several load and speed combinations, Fewer NO_x and particulate matter (PM) emissions are produced by PCCI, but higher CO and hydrocarbon (HC) emissions result. In addition, the nature of the PM differs from conventional combustion; the PM is smaller and has a much higher soluble organic fraction (SOF) content (68% vs. 30% for conventional combustion). Three catalyst technologies were studied to determine the affects of HECC on catalyst performance; the technologies were a lean NO_x trap (LNT), diesel oxidation catalyst (DOC), and diesel particulate filter (DPF). The LNT benefited greatly from the reduced NO_x emissions associated with PCCI. NO_x capacity requirements are reduced as well as overall tailpipe NO_x levels particularly at low load and temperature conditions where regeneration of the LNT is difficult. The DOC performance requirements for PCCI are more stringent due to the higher CO and HC emissions; however, the DOC was effective at controlling the higher CO and HC emissions at conditions above the light-off temperature. Below light-off, CO and HC emissions are problematic. The study of DPF technology focused on the fuel penalties associated with DPF regeneration or "desoot" due to the different PM loading rates from PCCI vs. conventional combustion. Less frequent desoot events were required from the lower PM from PCCI and, when used in conjunction with an LNT, the lower PM from less frequent LNT regeneration. The lower desoot frequency leads a \sim 3% fuel penalty for a mixture of PCCI and conventional loads vs. \sim 4% for conventional only combustion.

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1. Introduction

Further introduction of vehicles with lean engines such as the diesel engine into the marketplace can reduce petroleum consumption and greenhouse gas emissions, but emission regulations must be met to enable market introduction. Progress has been made on both combustion and catalyst control pathways to reduced emissions. For diesel engines, premixed charge compression ignition (PCCI) is a promising combustion technique that simultaneously reduces both NO_x and particulate matter (PM) emissions [1,2]. With respect to catalyst technologies, lean NO_x traps (LNTs), urea-

selective catalytic reduction (SCR), and diesel particulate filters (DPFs) have proven effective in controlling NO_x and PM emissions and have gained maturity in terms of understanding and commercial experience [3–7]. Both engine and catalyst improvements will affect the design of vehicle engine systems; thus, understanding the technical interactions between combustion and catalyst technologies is critical for optimizing the system.

A light-duty diesel engine (4-cylinder, 1.7-l Mercedes) has been operated in advanced combustion modes generally referred to as PCCI. PCCI combustion is achieved by increasing exhaust gas recirculation (EGR), advancing fuel injection timing, and increasing fuel rail pressure; these modifications lead to a more homogeneous combustion flame in the engine cylinder as opposed to the stratified flame that occurs along the fuel spray during conventional combustion. Under PCCI, the emissions from the engine change dramatically due to the homogeneous combustion. In general, fewer NO_x and particulate matter (PM) emissions are produced, but higher CO and hydrocarbon (HC) emissions result. PCCI can reduce the amount of NO_x and PM emissions required to be controlled by catalytic devices; thus, fuel penalties for active regeneration and costs of catalysts can be reduced. However, PCCI is difficult

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to achieve at high engine loads; this fact combined with cold start challenges and the higher CO and HC emissions leads to a scenario where catalysts will still be required. Therefore, understanding how the emissions from PCCI affect catalysts and emission control requirements is necessary. In the work presented here, the interaction of PCCI combustion with different catalyst technologies was studied

Three catalyst technologies were studied with PCCI combustion: lean NO_X trap (LNT), diesel oxidation catalyst (DOC), and diesel particulate filter (DPF). The LNT was studied at various engine load and speed conditions while the engine was operated with both PCCI and conventional combustion. Fuel efficiency and tailpipe emissions were characterized for varying regeneration frequencies. The DOC was studied to determine the effectiveness of the DOC for controlling the higher CO and HC emissions from PCCI. Finally, the DPF was loaded from PCCI and conventional combustion modes, and the affect of the lower PM from PCCI on desoot of the DPF was evaluated. The focus of the DPF study was on fuel consumption for the desoot process.

2. Experimental

2.1. PCCI combustion

A 4-cylinder 1.7-l Mercedes diesel engine was utilized for this study. The engine was operated with ultra low sulfur diesel (ULSD) fuel (<15 ppm S). The engine was operated with both conventional and PCCI combustion modes. A series of steady state load and speed conditions served as the test basis. During conventional operation, the engine calibration parameters defined by the original equipment manufacturer (OEM) were used. For PCCI operation, exhaust gas recirculation (EGR) was increased, fuel rail pressure was increased, and the timing of the main fuel injection was advanced [8]. These changes are expected to result in a more homogeneous fuel and air mixture in the cylinder at the point of ignition based on the literature [1].

The engine was operated on a 104 kW (140 hp) motoring direct current (DC) dynamometer. During operation, the fuel consumption of the engine was monitored with a gravimetric technique. The engine system fuel efficiency was defined by the amount of energy adsorbed by the dynamometer as useful work divided by the energy content of the fuel consumed for the engine and emission control system. The fuel penalty was defined as the amount of fuel used for active regeneration of the emission control device divided by the total engine system fuel use.

For control of the engine, the factory engine control module was replaced with a rapid development engine controller based on a dSpace® MicroAutoBox. This rapid development system provides complete control over all engine electronics, including timing, duration, and number of fuel injection events, intake throttle, EGR valve, and turbocharger wastegate. Modifications to the engine included the addition of an electronic intake throttle, an electronically controlled exhaust gas recirculation (EGR) valve (in lieu of the stock vacuum-operated valve), and an EGR cooler. These engine and control modifications were necessary to operate the engine in PCCI modes as well as to perform active regeneration of the LNT and DPF emission control technologies.

2.2. Catalysts

Experiments were conducted to study the effects of PCCI combustion on operation of lean NO_x trap (LNT), diesel oxidation catalyst (DOC), and diesel particulate filter (DPF) catalyst technologies. During the LNT study, the exhaust system included an upstream DOC for the purpose of removing oxygen from the

exhaust during the rich phase of the LNT lean–rich cycle. The DOC was a basic $100\,\mathrm{g/ft^3}$ Pt on $\mathrm{Al_2O_3}$ catalyst. A DPF was also in the exhaust system between the DOC and LNT catalysts. The DPF was a SiC substrate that was catalyzed with a proprietary precious metal loading. The LNT was a Ba-based prototype LNT formulation provided by the Manufacturers of Emissions Control Association (MECA). The LNT volume was 2.471. The DOC study included a catalyst manufactured by AirFlow Catalysts with $100\,\mathrm{g/ft^3}$ Pt and a proprietary formulation. The catalyst volume of the DOC was 1.241.The DPF study was performed with the same DOC, DPF, and LNT combination used for the LNT study. Here the volume of the DPF was 2.21.

2.3. Lean NO_x trap regeneration

In order to operate the LNT catalyst, a lean–rich exhaust cycle was generated by operating the engine at lean and rich air-to-fuel ratios; the rich operation enabled regeneration of the LNT for subsequent NO_x trapping. For all lean–rich cycle periods and combustion modes, the same regeneration parameters for the LNT were used. Regeneration was performed by throttling the engine intake and enriching the main fuel injection pulse to achieve an air-to-fuel ratio in the exhaust of 13.5 immediately upstream of the LNT catalyst as measured with an universal exhaust gas oxygen (UEGO) sensor. During enrichment of the main injection pulse, the timing of the main injection pulse was delayed by $\sim\!20$ crank angle degrees to avoid an excessive increase of torque during the regeneration event. The duration of the enrichment was 3 s. lean–rich periods in increments of 30 s (e.g. 30, 60, 90, and 120 s) were evaluated.

2.4. Diesel particulate filter regeneration

The differential pressure across the DPF was monitored during engine operation as an indicator of the status of the DPF. As more particulate accumulated on the DPF, the differential pressure increased to a point where regeneration of the DPF or "desoot" was necessary. A level of 0.6 in Hg was used as the standard trigger point for desoot operation based on data from early commercial systems that utilize DPFs [9]. In order to regenerate the DPF, excess fuel was added in the power stroke of the engine cycle at 80 crank angle degrees after top dead center. The excess fuel was only partially combusted and led to high HCs in the exhaust which oxidized over the DOC to heat the downstream DPF via the exothermic reaction over the DOC. The target temperature for the desoot operation was 600 °C at the DPF inlet. Differential pressure was monitored during desoot to determine when oxidation of the particulate matter on the DPF was completed; the typical period required for desoot was 12 min.

2.5. Emissions

Exhaust samples were acquired from the engine system and analyzed with a variety of techniques to quantify the different emission species. Criteria pollutants NO_x , CO, and HCs were measured by pulling raw exhaust through heated lines to analyzers for each species; the analyzers were Model 400-HCLD (chemiluminescence), Model 200 (non-dispersive infrared), and Model 300-HFID (flame ionization detector), respectively (all manufactured by California Analytical Instruments Models). PM was removed from the exhaust sample via Balston filters prior to the heated lines. The NO_x and HC analyzers were heated analyzers, and the CO analyzer operated at room temperature and required passing the gas sample through a chiller (Unique Products International Model 331-2876) to remove the H_2O from the sample.

Measurements of formaldehyde and acetaldehyde, which are Mobile Source Air Toxics (MSATs), were made by pulling dilute exhaust through a solid phase extraction cartridge coated with 2,4-dinitrophenylhydrazine (DNPH) (Waters Corp.); flow rate was maintained at 1 l/min through the cartridges. Subsequently, the DNPH derivatives were extracted and then analyzed using a liquid chromatograph (Hewlett-Packard 1100 HPLC) with ultraviolet (UV) detection. The eluent from the HPLC unit was transferred directly to a Bruker Daltonics® Esquire mass spectrometer where the hydrazone derivatives were identified using a negative electrospray ionization mass spectrometer (ESI/MS). HPLC separation was conducted using Restek Allure C18 column. More details appear in Storey et al. [10].

Exhaust particle size measurements were made following microtunnel dilution at $45\,^{\circ}$ C. Particle mean diameter, number–size distribution, surface area–size distribution, and total number concentration were measured by a scanning mobility particle sizer (SMPS; Model 3936, TSI Inc., St. Paul, MN). The SMPS includes a differential mobility analyzer (Model 3080) and condensation particle counter (Model 3025). Dilute exhaust and clean sheath air passed through the SMPS at 1 and 10 l/min, respectively. Data was acquired for particles with 7–300 nm electrical mobility diameter [10].

The soluble organic fraction (SOF) of particulate matter was determined by a solvent extraction method. Particulate matter is collected from dilute exhaust on Pallflex TX-40 TeflonTM coated quartz fiber filters. The filter is immersed in 20 ml of a mixture of 50% acetone and 50% hexane in a quartz-lined vessel. Subsequently, the filters are placed in a microwave accelerated reaction system (MARS; CEM Corp.). The temperature is increased to 115 °C and held for 10 min. This method was adapted from an EPA process for solvent extraction of soils contaminated with fuel hydrocarbons. Further information on the method can be found in Lewis et al. [11].

3. Results and discussion

3.1. PCCI combustion

Both the fuel efficiency and emissions during PCCI combustion are affected by combustion controlling parameters such as EGR, fuel rail pressure, and fuel injection timing. Fig. 1 shows the affect of EGR rate on the emissions and efficiency of PCCI operation; here efficiency is the amount of work produced by the engine per amount of energy in the fuel. The engine speed was $1500 \, \text{rpm}$, and the engine load was $2.6 \, \text{bar}$. For the data shown, PCCI injection timing and rail pressure were used. As EGR increases, NO_x emissions decrease, but CO and HC emissions increase. The emissions and efficiency change dramatically as EGR rates increase above 40%. As EGR rates

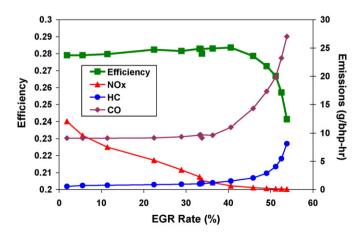


Fig. 1. Emissions of NO_x , CO, and HCs and efficiency during PCCI operation as a function of EGR rate.

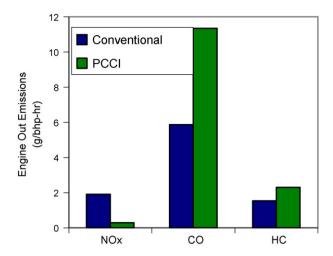


Fig. 2. NO_x, CO, and HC emissions for conventional and PCCI combustion.

increase, ultimately the fuel efficiency begins to plummet, and (not shown) engine operation becomes less stable. At the same point, CO and HC emissions rise due to the instability as incomplete combustion occurs. Thus, operation in PCCI is a balance between low NO_X and high CO and HC emissions; the optimal EGR rate is near the maximum fuel efficiency condition.

Fig. 2 shows a comparison of NO_x , CO, and HC emissions for PCCI as compared with conventional combustion; the engine speed and load were 1500 rpm and 2.6 bar, respectively. NO_x emissions are dramatically lower for PCCI combustion; however, CO and HC emissions are significantly higher. Fig. 3 shows data under the same conditions for two MSATs: formaldehyde and acetaldehyde. Both formaldehyde and acetaldehyde emissions are much higher during PCCI combustion in comparison to conventional combustion [10]. Thus, in addition to higher HC emissions from PCCI, the type of HC emissions that increase are MSATs.

Fig. 4 shows PM emissions for PCCI and conventional combustion at 1500 rpm and 2.6 bar. The PM emissions from PCCI are significantly lower than for conventional combustion. In addition, the nature of PM is quite different. The soluble organic fraction of PM for PCCI combustion is much higher. The size of PM from PCCI combustion is also generally smaller than from conventional combustion. Fig. 5 shows the size distribution of PM from PCCI and conventional combustion at 1500 rpm and 0.8 bar.

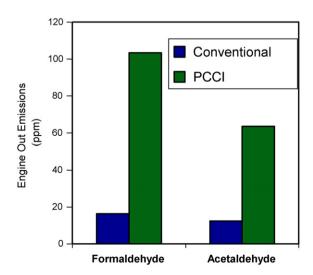


Fig. 3. Formaldehyde and acetaldehyde emissions from conventional and PCCI combustion.

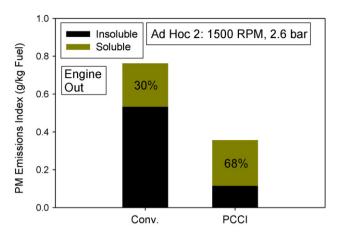


Fig. 4. PM emissions for conventional and PCCI combustion; the soluble organic fraction of PM is higher for PCCI combustion.

3.2. Lean NO_x trap (LNT)

As experiments were conducted with the LNT catalyst, the lean–rich cycle period was varied to enable a complete comparison between emissions and efficiency. As more frequent regeneration occurs, lower NO_x emissions results, but the fuel penalty for LNT operation increases and diminishes the overall fuel efficiency of the system. Thus, optimal system performance is a balance between NO_x emissions and fuel efficiency. By varying the lean–rich period during the experiments, the optimal conditions could be determined. Sweeps of the lean–rich period were conducted under operation with PCCI and conventional combustion. In addition to the conventional mode with OEM settings for EGR and injection parameters, another conventional mode with no EGR was evaluated as well. In this manner, three different combustion modes with three different engine out NO_x levels were compared.

Fig. 6 shows the NO_x emissions vs. engine system fuel efficiency for the two conventional combustion modes (no EGR and OEM level EGR) in comparison to PCCI combustion at 1500 rpm and 2.6 bar. For the graph, optimal performance is in the direction of the lower right corner where efficiency is maximized and NO_x emissions are minimized. The curves of performance for each combustion mode were generated by changing the LNT lean–rich period or regeneration frequency. As more frequent regeneration occurs, NO_x emissions decrease but so does the engine system fuel efficiency, which here includes fuel use by the engine during the lean and rich modes. Comparison between PCCI and the conventional combustion modes is somewhat subjective in this case. Lower NO_x emissions were achieved with PCCI combustion, but the engine system fuel effi-

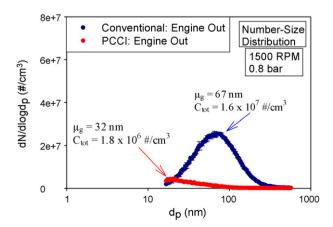


Fig. 5. Size distribution of PM for conventional and PCCI combustion.

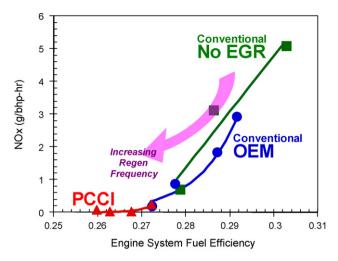


Fig. 6. NO_x emissions vs. engine system fuel efficiency at 1500 rpm and 2.6 bar; the system efficiency includes the fuel penalty for LNT regeneration.

ciency was the lowest for PCCI combustion as well. Since PCCI utilizes higher EGR rates, efficiency can decline, but the in-cylinder combustion differences due to the advanced timing and higher rail injection pressures can also affect efficiency. For the case in Fig. 6, the net efficiency changes cause a decrease in engine fuel efficiency as compared with conventional combustion.

Fig. 7 shows a similar comparison but at a different engine speed and load of 2000 rpm and 2.0 bar, respectively. At this engine condition, PCCI shows a clear advantage over the conventional combustion modes. PCCI gives lower NO_X emissions at the same engine system fuel efficiency as the conventional modes. Thus, in addition to the variations in engine system fuel efficiency for various lean–rich cycle parameters and combustion types, the efficiency changes with different engine load and speed parameters. Overall, the complex in–cylinder combustion process as well as the affects of EGR and LNT regeneration parameters all have bearing on the final engine system fuel efficiency.

Clearly, the lower NO_x emissions from PCCI combustion enable the LNT to achieve lower NO_x emissions from the engine system as compared with conventional combustion modes. However, the engine system fuel efficiency attained by the system varies with engine conditions. In some cases, PCCI efficiencies are comparable to conventional combustion modes, but for other points, PCCI shows a lower fuel efficiency than conventional combustion.

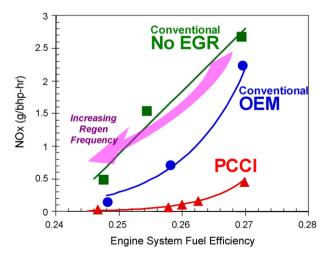


Fig. 7. NO_x emissions vs. engine system fuel efficiency at 2000 rpm and 2.0 bar; the system efficiency includes the fuel penalty for LNT regeneration.

3.3. Diesel oxidation catalyst (DOC)

The role of the diesel oxidation catalyst (DOC) technology with PCCI combustion will become more important as the higher CO and HC emissions from PCCI are required to be controlled. A DOC was evaluated to determine the oxidation efficiency for formaldehyde and acetaldehyde during PCCI combustion. Fig. 8 shows engine out and catalyst out formaldehyde and acetaldehyde emissions at three engine load and speed points. Engine out conventional (OEM) emissions are shown for reference as well. The three engine load and speed points resulted in catalyst temperatures of 119 °C, 220 °C, and 256 °C. Emissions are expressed as emissions index or mass of emissions per mass of fuel consumed. For reference, the Tier 2 Bin 5 regulation formaldehyde level is 0.24 g/kg fuel. As shown by the data, the low load condition of 1500 rpm and 1.0 bar gave the highest formaldehyde and acetaldehyde emissions, and PCCI emissions were much higher than the conventional OEM case. Furthermore, at the low catalyst temperature of 119 °C that resulted from the low load operation, the DOC was not effective at oxidizing the formaldehyde or acetaldehyde emissions. In contrast, at the other conditions of 2000 rpm and 2.0 bar and 1500 rpm and 2.6 bar, the DOC was able to control formaldehyde and acetaldehyde emissions to levels below the Tier 2 Bin 5 regulation level. These latter two engine conditions resulted in DOC catalyst temperatures above 200 °C. Thus, the DOC reduced MSAT emissions readily when suitable catalyst temperatures were attained, but below light-off temperatures, the MSAT levels from PCCI were higher than regulation levels.

3.4. Diesel particulate filter (DPF)

DPFs are common on diesel engine vehicles since the 2007 emission regulations for PM became in effect. Although the DPF technology has been very effective at reducing PM emissions, a fuel penalty is associated with the regeneration of the DPF. The regeneration event is also known as "desoot" and requires the DPF temperature to be raised to approximately 600 °C so that the trapped PM can oxidize. The frequency of the desoot events is often determined by the rise in backpressure across the DPF.

In the study here, the rate of rise in backpressure across the DPF was measured for various load and speed conditions. Conventional and PCCI combustion modes were studied, and a compilation of conventional only and multimode combustion data points were created to compare data sets. Here multimode indicates that both PCCI and conventional combustion modes were used to form the data set; this mixture of modes was used since at high loads, PCCI was not attained due to limitations in EGR rates at the higher loads. Specific load and speed points in the database were weighted based on the loads experienced in the FTP-75 transient driving cycle [12].

Fig. 9 shows the rate of rise in backpressure for both conventional and multimode data sets and the impact of the backpressure rise rate on fuel penalty and system efficiency. Fig. 9a shows the backpressure rise rate expressed in units of pressure per time based on a standard load and speed condition; the conventional data points show a much higher rise rate as compared with the multimode case. Based on a trigger level for the desoot operation of 0.6 in Hg, Fig. 9b shows the ensuing fuel penalty for the desoot frequency based on the backpressure rise rates shown in Fig. 9a. The calculations give a desoot frequency of once every 2.7 h for the conventional case compared with once every 4.2 h for the multimode case. The lower frequency of desoot events for the multimode case results in a lower fuel penalty of 3.1% vs. 4.3% for the conventional case. Finally, Fig. 9c shows the total engine efficiency given in BSFC units (brake specific fuel consumption) for both cases; the fuel consumption contribution due to desoot events is separated from the engine fuel consumption. The multimode case which contains both PCCI and conventional combustion modes benefits from the

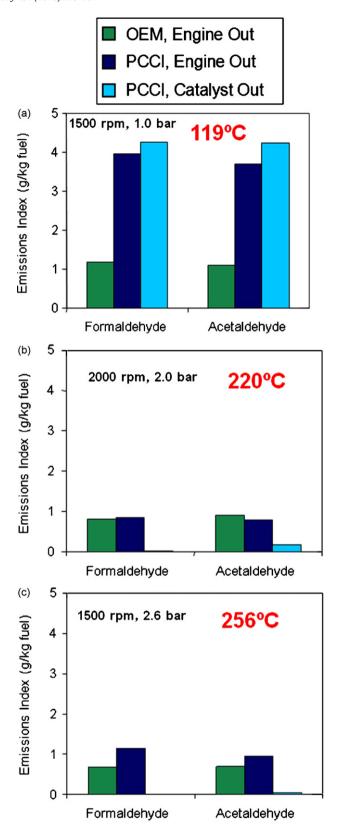


Fig. 8. Formaldehyde and acetaldehyde emission indexes for conventional (OEM) engine out and PCCI engine out and catalyst out samples at (a) 1500 rpm and 1.0 bar with 119 °C catalyst temperature, (b) 2000 rpm and 2.0 bar with 220 °C catalyst temperature, and (c) 1500 rpm and 2.6 bar with 256 °C catalyst temperature.

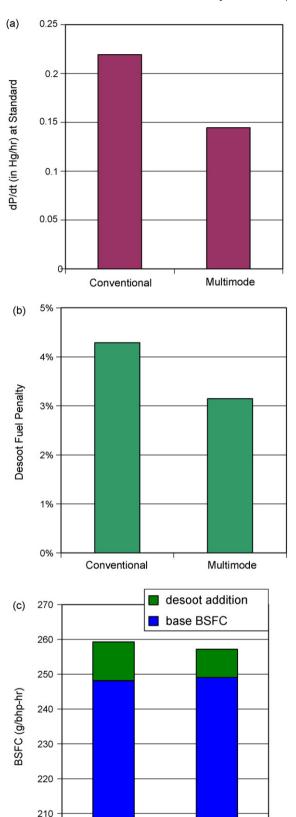


Fig. 9. Backpressure rise rate across the DPF (a), fuel penalty resulting in desoot operations with frequencies based on the backpressure rise rate (b), and system BSFC (c) for conventional and multimode combustion.

Multimode

Conventional

200

lower fuel penalty for desoot operations and gives a combined BSFC slightly better than experienced for conventional combustion only.

The data clearly shows that based on the parameters of the experiment presented here, the lower amount of PM from PCCI reduces the fuel penalty for DPF regeneration as compared with conventional only engine operation. However, there are important aspects of the PM generated in PCCI that may affect the fuel advantage with respect to DPF regeneration for other control algorithms and operating conditions. As shown, PCCI particulate is smaller in size and contains a higher soluble organic fraction as compared with PM from conventional combustion. The smaller size of the particulates from PCCI may affect the manner in which particulate loads onto the DPF substrate, and thereby, could potentially affect the differential pressure (used to trigger desoot) and the desoot event. Furthermore, the higher soluble organic fraction of the PCCI PM has the potential to affect the desoot event as well as the organic fraction may become volatile and oxidize at a different rate either during the ramp to desoot temperature or at the desoot temperature. The degree to which these size and composition aspects of the PCCI PM will affect the fuel penalty advantage is unclear and will require further study.

Another issue of relevance is the impact of the PCCI PM nature on future regulations. Number-based PM regulations will be implemented for Euro 5 standards in Europe in 2009 [13], and the smaller PM from PCCI may lead to a higher potential for PM slip past the DPF either during loading or desoot operation. Such, PM slip may contribute to high particulate count emissions and affect compliance with future number-base regulations. Furthermore, the volatilization of the soluble organic fraction of the PCCI PM could lead to HC emissions downstream which could affect tailpipe HC levels.

4. Conclusions

Experiments were conducted on a light-duty diesel engine to determine the effects of PCCI combustion on emission control catalysts. Data from conventional combustion was collected for comparison. PCCI results in lower NO_x and PM emissions but higher levels of CO and HCs. Formaldehyde and acetaldehyde (two MSATs) increase for PCCI as well. The catalyst technologies studied were LNTs, DOCs, and DPFs.

- LNTs generally benefited from PCCI combustion as the lower engine out NO_x levels resulted in even lower catalyst out emissions. The engine system fuel efficiency depended on the specific engine speed and load with some points resulting in similar efficiencies for PCCI and conventional combustion and other points showing slightly lower fuel efficiency for PCCI combustion.
- DOCs were generally efficient at oxidizing the increased levels of formaldehyde and acetaldehyde resulting from PCCI operation. However, at low loads where catalyst temperatures were less than 200°C, oxidation efficiencies were low and the increased formaldehyde and acetaldehyde emissions were not controlled.
- Lower PM emissions from PCCI benefited the DPF technology by lowering the frequency for desoot operations. Less desoot events lead to lower fuel penalties and better system fuel efficiency as shown by the comparison of sets of conventional combustion modes and a multimode case consisting of a mixture of PCCI and conventional combustions modes.

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