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Effect of Split Fuel Injection and EGR on NOx and PM Emission Reduction in a Low Temperature Combustion (LTC) Mode Diesel Engine

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<u>Research Highlights</u>

- Advancing SoMI and SoPI timings improved PCCI combustion
- Retarded SoMI timings resulted in higher NOx and PM emissions
- Increasing EGR reduced NOx and PM mass emissions simultaneously
- Increasing EGR rate effectively controlled the HRR of PCCI combustion
- Too high EGR resulted in higher HC and CO emissions



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2	Emission Reduction in a Low Temperature
3	Combustion (LTC) Mode Diesel Engine
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10 Abstract

11 In this study, an advanced combustion concept 'premixed charge compression ignition' 12 (PCCI) has been explored for diesel engines. PCCI combustion is a single-stage 13 combustion process, in which a large fraction of fuel burns in premixed combustion phase resulting in relatively lower in-cylinder temperatures compared to compression 14 ignition (CI) engine combustion. However at high loads, PCCI combustion results in 15 severe knocking and higher oxides of nitrogen (NOx) emissions. This limits the 16 applicability of this combustion concept to medium loads. This limitation of PCCI 17 18 combustion can be resolved by altering in-cylinder pressure-temperature history at the time of fuel injection. This can be also be resolved by deploying suitable split fuel 19 injection strategy and exhaust gas recirculation (EGR), which control combustion events 20 21 such as start of combustion (SoC) and combustion phasing, leading to lower knocking 22 and NOx emissions. To investigate the effects of various split injection strategy and EGR on PCCI combustion, engine experiments were conducted at different start of main 23 24 injection (SoMI) timings (12, 16, 20 and 24° bTDC), start of pilot injection (SoPI) timings 25 (30, 35 and 40° bTDC) and EGR rates (0, 15 and 30%). This study also included detailed

particulate characterization such as particulate number-size distribution using an 26 engine exhaust particle sizer (EEPS) and particulate bound trace metal analysis by 27 inductively coupled plasma-optical emission spectrophotometry (ICP-OES). PCCI 28 combustion was found to be superior at 35° bTDC SoPI timing and 15% EGR. At 29 retarded SoPI timing (30° bTDC), PCCI combustion resulted in slightly higher NOx and 30 particulate emissions, however at too advanced SoPI timing (40° bTDC), PCCI 31 32 combustion showed relatively inferior engine performance. Application of EGR improved PCCI combustion and emission characteristics, however at high EGR, PCCI combustion 33 resulted in inferior engine performance due to reduction in bulk in-cylinder 34 temperatures. Overall, this study showed that PCCI combustion stability, knocking and 35 NOx emissions can be optimized by selecting suitable combination of SoMI and SoPI 36 timings, and EGR rate. 37

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Keywords: Partially premixed charge compression ignition; Heat release rate; Exhaust
gas recirculation; Split injection; Knocking.

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42 <u>1. Introduction</u>

Rapid technological and economic advances in last few decades have culminated in 43 rapid depletion of petroleum resources. In transport sector, compression ignition 44 (CI) engines are being widely used currently, especially in light-duty and heavy-45 46 duty vehicles because of their higher thermal efficiency, greater reliability and 47 superior fuel economy compared to gasoline engines. However CI engines suffer 48 from major drawbacks of high oxides of nitrogen (NOx) and particulate matter (PM) emissions, which limit their applications due to prevailing stringent emission norms 49 50 globally. Trade-off between PM and NOx is the main challenge faced by CI engines. 51 The PM-NOx dilemma in CI engines was first addressed by Akihama et al. [1]. They

suggested that application of exhaust gas recirculation (EGR) might be one of the 52 possible solutions for this problem and experimentally studied the effects of ultra-53 54 high EGR on diesel combustion for simultaneous reduction in both NOx and PM. Too high EGR deteriorates the combustion characteristics and subsequently the 55 engine performance; therefore different researchers coupled EGR with advanced 56 combustion techniques such as homogeneous charge compression ignition (HCCI). 57 HCCI emerged in the late 1970's, when Onishi et al. [2] experimentally 58 demonstrated this novel combustion concept in a two-stroke engine. This concept 59 was further explored by Thring [3], and HCCI combustion was implemented in a 60 four-stroke engine. After these pioneering research efforts, several other researchers 61 including Christensen et al. [4], Stanglmaier et al. [5] and Maurya et al. [6] 62 successfully demonstrated HCCI combustion concept in spark ignition (SI) engines. 63 In 1990's, efforts were made to examine and deploy this concept in diesel engines. 64 Singh et al. [7] reported combustion characteristics of diesel HCCI engine. Even 65 66 though HCCI concept proved to be effective in reducing NOx emissions from diesel engines, there were significant unresolved issues related to start of combustion 67 68 (SoC), combustion phasing and, high hydrocarbons (HC) and carbon monoxide (CO) 69 emissions [8]. These challenges motivated researchers to develop a new low 70 temperature combustion (LTC) strategy, known as premixed charge compression ignition (PCCI) combustion. In PCCI combustion, fuel is injected at an intermediate 71 timing between that of HCCI and conventional CI combustion. Advanced start of 72 73 injection (SoI) timing results in a partially premixed fuel-air mixture due to 74 relatively lesser time available compared to HCCI combustion. Therefore, PCCI combustion can be considered as a 'premixed combustion phase dominated CI 75 combustion'. Due to low volatility of mineral diesel, diesel fuelled PCCI combustion 76 investigations mainly focused on high pressure direct fuel injection strategies 77

employing EGR [1, 9-12]. Higher fuel injection pressures and enhanced swirl ratios
promoted fuel-air mixing however sufficient premixing time between end of injection
(EoI) and SoC was necessary for achieving efficient PCCI combustion [13].

Initially, single stage direct injection of fuel was employed to achieve PCCI 81 82 combustion wherein early direct injection during the compression stroke promoted fuel-air mixing due to presence of higher in-cylinder temperature and longer charge 83 premixing time. However too advanced SoI timings resulted in fuel spray 84 impingement on the walls resulting in cylinder wall wetting, leading to incomplete 85 combustion and subsequently reduced thermal efficiency as well as higher HC 86 emissions [14-15]. In PCCI combustion, fuel-air mixture homogeneity was also 87 88 significantly affected by in-cylinder conditions (pressure-temperature history). For 89 controlling the in-cylinder conditions at the time of main injection, researchers employed split fuel injection. Hashizume et al. [14] proposed a concept of 'multiple 90 stage diesel combustion' (MULDIC), in which two-stage fuel injection was 91 implemented to achieve the LTC. Using MULDIC, they achieved significant 92 reduction in NOx and soot emissions simultaneously, however fuel economy was 93 94 inferior compared to conventional CI combustion. Neely et al. [15] investigated 95 effect of pilot injections (up to 3) to achieve PCCI combustion in light and heavy-96 duty vehicles. In case of single pilot injection, they observed considerable reduction in NOx emissions however higher CO emission. This CO penalty was reduced by 97 implementing multiple pilot injections. Effect of split injection strategy on NOx 98 99 formation was explored by Horibe et al. [16] and Torregrosa et al. [17]. They 100 reported that higher thermal efficiency and lower NOx emissions at moderate engine loads could be achieved by single pilot injection however excessive rate of 101 102 pressure rise (RoPR) limited the operating window of the PCCI combustion. In order to control the RoPR of PCCI combustion, researchers suggested using EGR. Higher 103

level of EGR was used to achieve longer ignition delay (to improve fuel-air mixing) 104 and lower in-cylinder temperature (to reduce NOx emissions) simultaneously [18]. 105 106 However very high level of EGR increased HC and CO emissions and reduced the 107 thermal efficiency. Kook et al. [19] and Kanda et al. [20] conducted experiments using different dilution rates (EGR) to attain PCCI combustion. High heat capacity 108 109 of diluting gas lowered the adiabatic flame temperature, which prevented NOx formation. These researchers reported that NOx and soot luminosity had direct 110 correlation with the adiabatic flame temperature and it decreased with increasing 111 EGR rate. Manente et al. [21] examined the physical and chemical concepts of EGR 112 on engine-out emissions in a PCCI engine. They reported that increasing EGR did 113 114 not affect engine efficiency however it decreased CO and HC emissions significantly. Detailed study of injection parameters and fuel spray impingement on emission 115 characteristics of mineral diesel fuelled PCCI engines was performed by Kiplimo et 116 al. [22]. They observed that an increase in fuel injection pressure (FIP) led to lower 117 118 HC, PM and NOx emissions with no change in CO emission. EGR stratification was a novel approach demonstrated by Andre et al. [23] and it was used to control rapid 119 120 heat release and combustion noise in a LTC engine. Jacobs et al. [24] and Hardy et al. [25] investigated lean PCCI combustion for controlling NOx and PM emissions 121 simultaneously. Lean PCCI combustion was achieved by employing high EGR rates, 122 higher FIP and SoI timings close to TDC. This strategy reduced NOx and PM 123 emissions because in-cylinder conditions were not favorable for formation of soot 124 particles in the combustion chamber in case of LTC. None of these studies discussed 125 126 effects of fuel injection parameters and EGR on particulate composition.

127 Many researchers showed that particulate emitted by PCCI combustion were 128 significantly lower therefore detailed particulates characterization remained 129 a rather ignored area by the researchers. However hypothesis of generating

negligible particulate from LTC was contradicted by Price et al. [26]. This was 130 supported by experimental studies of Kittelson and Franklin [27]. Agarwal et al. 131 [28] also undertook comprehensive experimental investigations to characterize 132 exhaust particulate from a mineral diesel fuelled LTC engine. It was amply 133 demonstrated without any doubt that the relative air-fuel ratio (λ) and EGR were 134 the major governing factors that affect particulate emissions from the LTC engine. 135 Further, the effect of intake air pressure and oxygen content of the inlet air on 136 particulate size-number distribution was investigated by Desantes et al. [29]. They 137 reported that a slight increase in inlet air oxygen content caused significant 138 reduction in CO, HC, and PM mass and particulate number emissions. Khalek et al. 139 140 [30] observed the influence of inlet air dilution (EGR) on particulate emissions from a mineral diesel fuelled HCCI engine. They reported that dilution air temperature, 141 dilution ratio and relative humidity were quite important for the formation of 142 nucleation mode particulate ($D_p < 50$ nm). However accumulation mode particulate 143 144 formation was less dependent on dilution conditions. Idicheria et al. [31] examined soot formation in PCCI combustion at very high EGR rates and reported that an 145 146 increase in ambient temperature resulted in higher soot formation in presence of high EGR rate compared to no EGR case. Researchers also reported that particulate 147 composition was different in case of LTC compared to CI combustion [28], due to 148 different combustion characteristics of LTC. Among composition of particulate, trace 149 metals, polycyclic aromatic hydrocarbons (PAHs) and benzene soluble organic 150 fraction (BSOF) content are important. Springer [32] carried out experiments to 151 evaluate particulate bound trace metals from light-duty and heavy-duty diesel 152 engines. He reported that presence of trace metals like calcium, sodium, 153 phosphorus, zinc, silicon, etc., were strongly affected by in-cylinder conditions 154 during combustion. Agarwal et al. [28] also investigated particulate bound trace 155

metals from mineral diesel fuelled LTC engine. They reported that most of trace metals mainly originated from incomplete combustion of fuel (trace metals in fuel), wear of engine components and pyrolysis of lubricating oil (from organo-metallic additives). However detailed analysis of particulate such as trace metals emitted from PCCI engines has not been thoroughly investigated.

161 All these studies indicated that fuel injection timing, strategy and charge dilution affect 162 combustion, performance, emissions and particulate characteristics of a LTC engine. These studies were carried out by considering variations in each parameter separately. 163 However combined effect of these parameters was not explored. This study evaluates the 164 165 effects of split injection and EGR on combustion, performance, emissions and particulate 166 characteristics simultaneously. The experiments were carried out in a single cylinder 167 research engine operated in PCCI combustion mode. Detailed particulate characterization including particulate number-size distribution and particulate bound 168 trace metal analysis was done. These are the innovative aspects of this experimental 169 170 investigation, which were not been explored by previous studies given in open literature. To support the particulate characterization results, detailed analysis of combustion, 171 172 performance and emission characteristics of PCCI combustion has been also carried out as well. Effects of SoPI and SoMI timings and EGR on NOx-PM trade-off is another 173 important aspect of this study. 174

175

176 <u>2. Experimental Setup</u>

In this experimental study, a single cylinder direct injection compression ignition (DICI) research engine (AVL List GmbH; 5402) was used to perform PCCI experiments. This test engine was a single cylinder version of a four-cylinder automotive high-speed direct injection (HSDI) diesel engine and was equipped with a modern common rail direct injection (CRDI) system. The mechanical dynamics of the engine was made similar to a

multi-cylinder engine using first order force balancers. A transient (AC) dynamometer 182 (Wittur Electric Drives GmbH, 2SB-3) was used to control the engine speed and torque. 183 184 The engine was equipped with a fuel measurement unit, a fuel conditioning unit, a 185 chiller unit, a coolant conditioning system and a lubricating oil conditioning system for carrying out all investigations under controlled experimental conditions. During entire 186 187 experiment, the lubricating oil and fuel temperatures were maintained at 90° and 25°C 188 respectively. For combustion analysis, a water-cooled piezoelectric pressure transducer (AVL, QC34C) was installed in the engine cylinder head. Rotation of the crankshaft was 189 monitored using an optical encoder (AVL, 365C). Cylinder pressure-crank angle data 190 191 was acquired and analyzed by a high speed combustion data acquisition system (AVL, 192 IndiMicro). Schematic of the experimental setup is shown in Figure 1 and the technical specifications of the engine are given in Table 1. 193

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Figure 1: Schematic of the experimental setup

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Table 1: Technical specifications of the test engine

196 Engine management system (EMS) of this engine had flexibility to control and measure 197 fuel injection parameters in manual mode of operation. Flexible fuel injection system of 198 EMS was capable of employing 4 injections in a cycle, including 2 pilots, 1 main and 1 199 post injection. An open loop fuel injection control strategy was loaded in the ETAS system to control fuel injection parameters independently. This control system consisted 200 of an electronic control unit (ECU), a communication interface (ETAS, ETK 7.1) and an 201 INCA software program. The injection parameters for each injection event could be 202 203 modified and logged independently through the INCA software, which was used to 204 communicate with the ETAS system.

To control PCCI combustion, a fraction of exhaust gas (coming directly from the engine) was recirculated back into the intake manifold. For controlling the EGR, a control valve was installed in the EGR loop. EGR rate was measured by reduction in mass flow rate of

fresh intake air since reduction in mass flow rate of fresh air was directly proportional 208 209 to the EGR. Quantity of fuel supplied to the engine was measured using a Coriolis force 210 based fuel metering unit (AVL, 733s). This system performs continuous measurement of weight of a measuring vessel, through which fuel is supplied to the engine. To measure 211 gaseous emission concentrations, a raw exhaust emission analyzer (Horiba, ESXA-1500) 212 was used. This equipment comprised of a CO/ CO_2 analyzer (NDIR detector: MCA-213 220UA), O₂ analyzer (Paramagnetic pressure detector: MCA-220UA), HC analyzer (Hot 214 flame ionization detector: FIA-225UA) and NO_x analyzer (Chemiluminescense detector: 215 CLA-220UA). Opacity of exhaust was measured by a smoke opacimeter (AVL; 437). 216 217 Particulate emission characterization was done using an engine exhaust particle sizerTM (EEPS) (TSI Inc.; 3090), which was capable of measuring particle sizes ranging from 5.6 218 - 560 nm and particle concentrations up to 10⁸ particles/ cm³ of exhaust gas. For 219 particulate composition analysis, a partial flow dilution tunnel was used to collect the 220 particulate emitted by the engine on a preconditioned filter paper. Particulate loaded 221 222 filters were analyzed for trace metals using inductively coupled plasma optical emission spectrophotometer (ICP-OES) (Thermo Fischer Scientific, iCAP DUO 6300 ICP 223 224 Spectrophotometer).

225

226 <u>3. Results and Discussion</u>

227 Objectives of this study were to select a suitable split injection strategy and optimum 228 EGR rate, which could deliver lower NOx and PM emission and control the engine 229 knocking. To attain this objectives, PCCI experiments were performed at varying SoPI 230 timings (30, 35 and 40° bTDC), SoMI timings (12, 16, 20 and 24° bTDC) and EGR rates 231 (0, 15 and 30%). During entire set of experiments, FIP and engine speed were 232 maintained constant at 700 bar and 1500 rpm respectively and mineral diesel was used 233 as test fuel. Results obtained from the experiments were divided into five categories

namely: combustion, performance, emissions, particulate characteristics and particulate
bound trace metals and the main outcome of this study was summarized as statistical
plots between PM and NOx emissions.

237

238 3.1 Combustion Characteristics

Parameters such as in-cylinder pressure history, heat release rate (HRR), SoC, etc., are very effective tools for analyzing the engine combustion characteristics. In this study, pressure-crank angle data was acquired by a high speed data acquisition system. To eliminate cycle-to-cycle combustion variability, average data set of 250 consecutive engine cycles was used for detailed combustion analysis.

Figure 2: Variations in cylinder pressure and HRR w.r.t. crank angle at different SoPI
and SoMI timings

Figure 2 shows the variation in cylinder pressure and HRR at different SoPI and SoMI 246 timings. At each SoPI timing, SoMI timings sweep was taken from 12 to 24° bTDC. 247 248 During experiment, 15% EGR rate was maintained. Results obtained showed that advancing SoMI timing improved PCCI combustion due to longer time availability for 249 250 fuel-air mixing. At advanced SoMI timings (20 and 24° bTDC), peak in-cylinder pressure (P_{max}) and peak HRR increased and shifted towards bTDC. This indicated higher 251 premixed combustion tendency at advanced SoMI timings. At advanced SoMI timings, 252 main combustion duration also reduced (reduced HRR curve width) due to faster fuel-air 253 chemical kinetics. These trends are similar to those reported by Zhao et al. [33]. 254 Advancing SoPI timings affected PCCI combustion in two ways: (i) advanced SoPI 255 timings provided longer time for in-cylinder conditioning, which resulted in 256 257 homogeneous fuel-air mixture and improved PCCI combustion, and (ii) too advanced SoPI timings led to inferior fuel-air mixing due to lower in-cylinder temperature and 258 pressure. In presence of lower in-cylinder temperature, fuel vaporization decreased. 259

However lower in-cylinder pressure deteriorated fuel spray characteristics (relatively 260 bigger fuel droplets leading to longer spray tip penetration and smaller spray area), 261 which ultimately affected fuel-air mixing characteristics [34]. Dominantion of these two 262 factors can be clearly seen from the trends for in-cylinder pressure. At 30° bTDC SoPI 263 timings, less time availability for in-cylinder conditioning resulted in slightly lower 264 P_{max}, higher HRR and higher RoPR (steeper in-cylinder pressure curves). At 40° BTDC 265 SoPI timing, slightly inferior in-cylinder conditions dominated over the time availability 266 factor, resulting in lower P_{max}, HRR and RoPR (flatter in-cylinder pressure curves). 267 Ganesh et al. [35] performed similar experiments and observed similar combustion 268 characteristics. Amongst all SoPI timings, 35° bTDC showed trade-off between the above 269 two factors, which resulted in slightly higher (~2-3 bar) P_{max} compared to 30 and 40° 270 bTDC. With advancing SoPI timings, slightly advanced SoC was another important 271 observation. This indicated that SoPI timing controlled the chemical kinetics of the fuel-272 air therefore it can be used to control PCCI combustion. 273

Figure 3 shows the variation in cylinder pressure and HRR at different EGR rates and SoMI timings. At each EGR rate, SoMI timings were varied from 12 to 24° bTDC. During these experiments, SoPI timing was maintained constant at 35° bTDC. Variations in combustion characteristics at different SoMI timigs were similar to those observed in case of varying SoPI timings, however effects of varying SoMI timings were greater at higher EGR rates. This was mainly due to relatively lesser fuel quantity and lower in-cylinder temperatures at higher EGR rates.

Figure 3: Variation in cylinder pressure and HRR w.r.t. crank angle for different SoMI timings and EGR rates

Results obtained showed that P_{max} and maximum HRR decreased with increasing EGR rate. Exhaust gas consists of primarily inert species therefore increasing EGR rate reduced the oxygen content of intake air, resulting in relatively lower chemical kinetics

of fuel-air mixtures. Presence of gaseous species with high heat capacity such as CO_2 , 286 water vapor, etc., in exhaust gas led to absorption of combustion generated heat thus 287 lowering the P_{max} and HRR. This is the main reason for lower NOx formation at higher 288 EGR rates. Retarded SoC with increasing EGR rate was another important observation 289 of this study. With increasing EGR rate, presence of inert species in the exhaust gas led 290 291 to longer ignition delay and subsequently retarded the SoC timings. Effect of EGR rate 292 on combustion stability and knocking characteristics can also be observed from the trends of cylinder pressure and HRR. At 0% EGR rate, HRR was too high, which led to 293 noisy combustion. With increasing EGR rate, combustion knock reduced. However at 294 very high EGR rate (~30%), combustion became too slow, which deteriorated the PCCI 295 296 engine performance and resulted in higher HC emissions. Amongst all the three EGR rates, 15% EGR rate was found to be the most suitable for PCCI combustion because it 297 298 exhibited a trade-off between combustion and performance characteristics.

299 Figure 4: SoC, combustion phasing and combustion duration w.r.t. SoMI timings at

different (a) SoPI timings and (b) EGR rates

Figure 4 (a) shows variation in SoC, combustion phasing and combustion duration at
different SoMI and SoPI timings. These parameters were calculated from mass fraction
burned (MFB) analysis. MFB was calculated by Rossweiler and Withrow method [36] as
given below:

$$(\Delta p_c) = p_i - p_{i-1} (\frac{V_{i-1}}{V_i})^{\gamma}$$

305

300

306 Here Δp_c is the increase in cylinder pressure due to combustion and γ is the polytropic 307 exponent. Using this relation, MFB can be computed as:

$$\frac{m_{b(i)}}{m_{b(total)}} = \frac{\sum_{j=0}^{i} \Delta(p_c)_j}{\sum_{j=0}^{N} \Delta(p_c)_j}$$

Here it is assumed that sample 0 is between inlet valve closing and SoC and sample N isafter the completion of combustion.

311 In the current study, crank angle position corresponding to 10% MFB (CA₁₀) was considered as SoC. In PCCI combustion, combustion started well before TDC (~2-10° 312 bTDC) due to advanced SoMI timings and faster chemical kinetics of fuel-air mixture. 313 Advancing SoMI timing from 12 to 24° bTDC also resulted in advanced SoC. This trend 314 was also visible from cylinder pressure and HRR curves. Advancing SoPI timings 315 resulted in slightly advanced SoC. This was attributed to improved fuel-air mixing due 316 317 to longer time availability. The difference between SoC timings at different SoPI timings 318 increased at advanced SoMI timings. This showed that advanced SoPI timing was more 319 effective at advanced SoMI timings (~20-24° bTDC) compared to retarded SoMI timings (~12-16° bTDC). 30 and 35° bTDC SoPI timings resulted in almost similar SoC, however 320 40° bTDC SoPI timing resulted in slightly advanced SoC. This showed that chemical 321 kinetics of fuel-air mixture was not significantly affected by fuel-air premixing, but was 322 323 significantly affected by in-cylinder conditions. This could be clearly observed from the 324 combustion phasing results. Crank angle position corresponding to 50% MFB (CA_{50}) was 325 taken as combustion phasing. Combustion phasing affected PCCI combustion efficiency, 326 which decreased for too advanced as well as too retarded combustion phasing. Advanced combustion phasing led to higher HRR which resulted in excessive knocking. However 327 late combustion phasing led to inferior combustion, which resulted in higher HC and CO 328 329 emissions. Combustion phasing also followed similar trend at different SoMI and SoPI 330 timings as that of SoC. However differences between combustion phasing at different 331 SoPI timings were relatively lower compared to that of SoC. In PCCI combustion, combustion phasing was significantly advanced compared to CI combustion [37]. This 332 was attributed to dominance of premixed combustion phase, which resulted in relatively 333 faster combustion compared to CI combustion. Combustion duration is defined as the 334

crank angle difference between 10 and 90% MFB (CA₉₀ - CA₁₀). In PCCI combustion, 335 variation in combustion duration shows the rapidness of combustion. Results obtained 336 337 showed that combustion duration of PCCI combustion (~10-20 CAD) was significantly shorter compared to CI combustion (~30-40 CAD). This was mainly due to absence of 338 diffusion combustion phase (slower combustion) in PCCI mode. With advanced SoMI 339 timings, combustion duration slightly decreased. This trend also validated previous 340 observation of relatively faster chemical kinetics of fuel-air mixture at advanced SoMI 341 timings. Combustion duration slightly decreased at advanced SoPI timings though the 342 difference was not significant. At all SoPI timings, combustion duration varied from 343 344 ~12-17 CAD.

345 Figure 4 (b) shows the variation in SoC, combustion phasing and combustion duration at different SoMI timings and EGR rates. In the experiment, SoPI timing was maintained 346 constant at 35° bTDC. At 0% EGR rate, SoC was significantly advanced compared to 15 347 and 30% EGR rates. This was mainly due to presence of relatively higher fuel quantity, 348 349 which enhanced chemical kinetics of fuel-air mixtures, resulting in advanced SoC. 350 Combustion phasing also varied similar to SoC. Increasing EGR rate led to relatively advanced combustion phasing. These observations showed that EGR affected both, the 351 352 fuel-air mixing (hence SoC), as well as the chemical kinetics of fuel-air mixture (i.e. combustion phasing). At 30% EGR rate, combustion phasing retarded due to slower 353 chemical kinetics of fuel-air mixture. At higher EGR rates, presence of inert gaseous 354 species reduced the reaction kinetics of fuel-air mixture and reduced the in-cylinder 355 356 temperature further, thus retarding the combustion phasing. With increasing EGR rate, 357 combustion duration slightly increased, however the difference in combustion duration 358 at different EGR rates was negligible. Combustion duration in PCCI combustion was controlled by two factors: (i) with increasing EGR rate, slower fuel-air chemical kinetics 359 increased the combustion duration, and (ii) presence of lower fuel quantity decreased the 360

361 combustion duration. Due to these two counter effects of EGR, combustion duration
362 remained almost constant for different EGR rates. The results obtained by Hardy et al.
363 [25] were also similar to these findings. Figure 5 shows the variation in knocking
364 integral (KI), knock peak (KP) and combustion noise at different SoPI timings and EGR
365 rates.

KI is the integral of superimposed, rectified knock oscillations and KP reflects absolute maxima of the rectified knock oscillations superimposed on the in-cylinder pressure traces. To calculate these parameters, in-cylinder pressure signal was filtered through a high pass filter and then rectified. Parameters such as KI or KP of the superimposed oscillations were determined from these signals. Cylinder noise levels were calculated from the cylinder pressure signals.

Figure 5 (a) shows the variations in KI, KP and combustion noise w.r.t. SoMI and SoPI 372 timings. In PCCI combustion, KI has been shown to be very low compared to CI or HCCI 373 combustion [38] and this was attributed to presence of pilot fuel injection, which 374 375 improves fuel-air mixing due to higher in-cylinder temperatures. In this study, application of EGR further improved the PCCI knocking characteristics due to relatively 376 377 slower chemical kinetics of fuel-air mixtures. With advancing SoMI timing, KI slightly decreased with almost negligible variations. Advancing SoPI timing didn't affect KI 378 significantly. 379

Figure 5: Variation in knock integral, knock peak and combustion noise w.r.t. SoMI
timings at different (a) SoPI timings and (b) EGR rates

Similar to KI, KP was also low for PCCI combustion. Advancing SoMI or SOPI timings also did not affect KP significantly, though it decreased slightly. This was attributed to improved fuel-air mixing. Advancing SoMI timing resulted in slightly higher cylinder noise, however variation of SoPI timing didn't affect combustion noise. These results showed that variations in SoI timings didn't affect knocking characteristics. Knocking

characteristics of PCCI combustion at different SoPI and SoMI timings showed that 35°
bTDC resulted in slightly stable combustion compared to relatively advanced (30° bTDC)
or retarded (40° bTDC) SoPI timings. This was mainly due to trade-off between incylinder conditions and time availability for fuel-air mixing, which directly influenced
combustion phasing.

Figure 5 (b) shows the variations in KI, KP and combustion noise at different SoMI 392 393 timings and EGR rates. KI slightly decreased with advancing SoMI timings. Increasing 394 EGR reduced KI, which reflected smoother combustion at higher EGR rates. This observation was further validated by KP results. As EGR rate increased from 0 to 30%, 395 KP decreased from ~8 to ~2 bar. This was mainly due to dilution effect of EGR, which 396 397 directly controlled the chemical kinetics of fuel-air mixture. At higher EGR rates, lower in-cylinder temperatures also suppressed knocking. Cylinder noise was also significantly 398 affected by EGR. With increasing EGR rates from 0 to 30%, combustion noise 399 continuously decreased from ~98 to ~92 dB. Comparison of PCCI combustion results at 400 401 different EGR rates indicated that EGR played an important role in PCCI combustion thus showing its potential for noise and knock reduction. However too high EGR 402 adversely affected the performance of PCCI engines and resulted in higher HC and CO 403 404 emissions.

405

406 **3.2 Performance Characteristics**

To investigate the effects of split injection and EGR on PCCI engine performance, experiments were carried out at varying SoPI timings and EGR rates. In this study, brake thermal efficiency (BTE), brake specific fuel consumption (BSFC) and exhaust gas temperature (EGT) were measured and plotted w.r.t. SoMI timings. At each experimental condition, performance parameters were measured three times and average was presented with error bars.

Δ	1	3
-	-	J

4	1	4

414 Figure 6: Variations in BTE, BSFC and EGT w.r.t. SoMI timings at different (a) SoPI 415 timings and (b) EGR rates

Figure 6 (a) shows the variations in PCCI engine performance parameters at varying 416 SoPI and SoMI timings. Results obtained show that BTE decreased with advancing 417 SoMI timings. This was mainly due to dominant premixed combustion phase, which led 418 to relatively higher negative piston work, resulting in lower BTE. Advancing SoPI 419 timing from 30 to 35° bTDC resulted in slightly higher BTE, but further advancing SoPI 420 timing (up to 40° bTDC) decreased BTE drastically. With retarded SoPI timing (30° 421 bTDC), lesser time availability for fuel-air mixing led to inferior combustion. However 422 423 with advanced SoPI timing (40° bTDC), lower peak cylinder pressure and temperature both dominated, resulting in inferior combustion. BSFC followed similar behavior at 424 different SoMI and SoPI timings, with lowest BSFC attained at intermediate SoPI (35° 425 bTDC) and retarded SOMI (12° bTDC) timing. EGT was measured very close to the 426 427 exhaust port. EGT gives qualitative information of in-cylinder combustion. In PCCI combustion, EGT was observed to be significantly lower (~100°C) compared to CI 428 429 combustion [39] and was attributed to absence of diffusion combustion. Application of 430 EGR was another important reason for lower EGT in PCCI combustion mode. In this study, EGT slightly reduced with advanced SoMI and SoPI timings. This was due to 431 longer time availability, which improved fuel-air mixing and promoted premixed 432 combustion. Negligible diffusion combustion with slightly lower EGT was observed. 433 Amongst the three SoPI timings, 35° bTDC showed minimum EGT (~225°C). 434

Figure 6 (b) shows variation in engine performance parameters at different SoMI 435 timings and EGR rates. BTE decreased with increasing EGR rate. This was mainly due 436 to two reasons: (i) lower fuel quantity at higher EGR rates, which retarded the chemical 437 kinetics of fuel-air mixture, resulting in slightly inferior combustion, and (ii) lower in-438

cylinder temperature due to presence of higher heat capacity exhaust gas, which 439 encouraged incomplete combustion. These factors resulted in higher CO and HC 440 441 emissions and adversely affected PCCI engine performance. BSFC followed a similar trend. BSFC continuously increased with increasing EGR rate. Effect of EGR was also 442 seen by variations in EGT. EGT drastically decreased (by up to 75°C) with increasing 443 EGR rate. This is the main advantage of PCCI combustion because lower EGT 444 represents absence of diffusion combustion phase because thermal NOx formation takes 445 place during diffusion combustion phase. Engine performance results showed that 446 increasing EGR rate slightly decreased the PCCI engine performance however 447 significant reduction in EGT occurred at 15% EGR rate. This shows a trade-off between 448 reduction in BTE and EGT, therefore it can be considered as optimized EGR rate for 449 PCCI combustion in the present experiment. 450

451

452 3.3 Emission Characteristics

To compare the PCCI mode engine emission characteristics, CO, HC, NOx and smoke opacity were measured at different SoPI timings (30, 35 and 40° bTDC) and EGR rates (0, 15 and 30%). CO, HC and NOx emissions are presented as brake specific mass emissions (g/kWh) and smoke opacity is measured in absolute units.

457 Figure 7: Variations in mass emissions of CO, HC, NOx and smoke opacity w.r.t. SoMI
458 timings at different (a) SoPI timings and (b) EGR rates

Figure 7(a) shows variations in CO, HC and NOx emissions, and smoke opacity w.r.t. SoMI timings at different SoPI timings. In IC engines, CO and HC are formed mainly due to incomplete combustion. Other researchers have also reported slightly higher CO and HC emissions from PCCI combustion mode [23-25]. CO is an intermediate combustion product, primarily formed due to incomplete oxidation of CO to CO_{2} , under relatively lower in-cylinder temperature conditions. Advanced SoMI timings lead to

relatively lower CO emissions. Relatively advanced combustion phasing at advanced 465 SoMI timings was the main reason for this behavior. Results showed that CO emission 466 467 increased slightly in case of advancing the SoPI timing from 30 to 35° bTDC. At 468 advanced SoPI timings, improved fuel-air premixing prevented diffusion combustion, leading to relatively lower in-cylinder temperature. With further advancing SoPI timing 469 from 35 to 40° bTDC, CO emission slightly decreased. This was attributed to slightly 470 471 inferior in-cylinder conditions, which promoted diffusion combustion therefore lower CO emissions. Similar to CO emissions, HC emissions were also observed to be higher in 472 PCCI combustion mode. In IC engines, HC formation takes place due to three reasons: 473 (i) incomplete combustion (shorter combustion duration), (ii) trapped fuel droplets in 474 475 crevice volume (early injection at higher FIPs), and (iii) in-cylinder wall quenching (lower in-cylinder temperature). Results obtained show that HC emissions increased 476 with advancing SOMI and SoPI timings. Advancing SoI timings result in homogeneous 477 fuel-air mixture, which promotes premixed combustion. This leads to lower in-cylinder 478 479 temperature and forms HCs due to incomplete combustion and wall quenching. With 480 advanced SoI timings, relatively larger fraction of fuel enters into the crevice volume 481 resulting in higher HC emissions. Fuel spray impingement at advanced SoI timings may 482 be another reason for higher HC emissions, wherein fuel spray comes in contact with cold in-cylinder walls and combustion is quenched. Higher HC emissions also affect 483 combustion efficiency adversely, which in turn reduce overall thermal efficiency. Ultra-484 low NOx emission is the main advantage of PCCI combustion. NOx formation mainly 485 486 occurs in diffusion combustion phase, where in-cylinder temperatures are too high. In 487 PCCI combustion, absence of a prominent diffusion combustion phase is the prime reason for lower NOx formation. NOx emissions increased slightly with advanced SoMI 488 timings. Amongst all three SoPI timings, lowest NOx was obtained for 35° bTDC. This 489 was the main reasons for selecting 35° bTDC as the optimum SoPI timing in further 490

experiments. Smoke opacity reflects qualitative pollutant level in the exhaust gas. 491 Lower smoke opacity is another advantage of PCCI combustion. Results showed that 492 493 smoke opacity decreased with advancing SoMI timings. Improved fuel-air mixing due to longer time availability was the main reason. Advancing SoPI timing first reduced 494 smoke opacity, however too advanced SoPI timing resulted in slightly higher smoke 495 opacity. Higher smoke opacity at 40° bTDC SoPI timing can be correlated to higher HC 496 497 emissions. Higher HC emissions promoted more soot nuclei formation, which resulted in higher smoke opacity. Lowest smoke opacity at 35° bTDC SoPI timing makes it the most 498 favorable condition for PCCI combustion mode. 499

Figure 7(b) shows the variation in CO, HC and NOx emissions, and smoke opacity at 500 501 varying SoMI timings and EGR rates. Results obtained showed that CO and HC emissions increased with increasing EGR rates. At higher EGR rate, in-cylinder 502 temperature became too low, which reduced oxidation of CO to CO2, leading to higher 503 CO emissions. At 30% EGR rate, availability of oxygen further reduced, resulting in 504 505 increased CO emission. CO emission can also be related to the retarded combustion phasing, which resulted in slower chemical kinetics of fuel-air mixture, inhibiting CO to 506 507 CO_2 conversion. With increasing EGR rate, in-cylinder temperature became too low to 508 oxidize the fuel completely which increased the unburned HC emissions. Combustion temperature near the cylinder walls was even lower due to higher heat losses. Therefore 509 at locations in the vicinity of cylinder walls, combustion was either quenched or did not 510 occur at all, which further increased the HC emissions. NOx formation was found to be 511 sensitive to EGR. With increasing EGR rate, NOx emissions reduced continuously. 512 These observations were in agreement with that of variations in EGT (Figure 6(b)). 513 Increasing EGR rate from 0 to 15% resulted in ~60% reduction in NOx emissions. 514 Further increase in EGR rate led to even lower NOx emissions, but it also caused 515 inferior and erratic engine performance. Therefore 15% EGR rate was considered as a 516

reasonable trade-off between the engine performance and the emission characteristics. 517 Smoke opacity slightly increased with increasing EGR rate, which led to lower in-518 519 cylinder temperatures. At higher EGR rate, lower in-cylinder temperatures promoted soot formation and enhanced smoke opacity. Overall emission results reflected that 520 increasing EGR rate resulted in slightly higher CO, and HC emissions and smoke 521 opacity, and these increments were relatively lower at 15% EGR rate compared to 30% 522 EGR rate. Therefore 15% EGR was used for optimizing PCCI engine performance and 523 emission characteristics. 524

525

526 3.4 Particulate Characteristics

527 To compare the characteristics of particulate emitted by diesel fuelled PCCI engine, two parameters used were: (i) Particulate number-size and (ii) Particulate surface area-size 528 distributions. Particulate number-size distribution was determined after thermal 529 stabilization of the engine. Particulate sampling was done for one minute at a sampling 530 531 frequency of 1 Hz. Average of these 60 data points were analyzed and presented along with standard deviation as the error bars, in the following figures. Figure 8 shows the 532 533 number-size and surface area-size distributions of particulate at varying SoPI and SoMI 534 timings, and 15% EGR rate.

Figure 8: (a) Number-size and (b) Surface area-size distributions of particulate at
varying SoPI and SoMI timings, and 15% EGR rate

Variations in particulate number-size distributions with SoPI and SoMI timings can be correlated with two parameters, namely (i) in-cylinder conditions (temperature and pressure), and (ii) time availability (for fuel-air mixing). Trends clearly indicated that particulate number concentration at a given size decreased with advancing SoMI timings. This was mainly due to relatively longer time available for fuel-air mixing, which resulted in formation of more homogeneous mixture. PCCI combustion at

advanced SoMI timings shifted peak particulate number-size distribution towards 543 larger particulate. This showed higher adsorption of condensed exhaust species on 544 545 primary particles. With advanced SoPI timing, particle number concentration first decreased (from 30 to 35° bTDC) and then increased (from 35 to 40° bTDC). Advancing 546 SoPI timing from 30 to 35° bTDC decreased particulate number concentration, however 547 548 peak of particulate number size-distribution shifted towards larger particles. Effect of variation of SoMI timing was also relatively more significant at 35° bTDC, which 549 resulted in slightly lower in-cylinder temperature due to improved fuel-air pre-mixing. 550 551 Lower in-cylinder temperature enhanced particulate agglomeration, leading to larger particles in relatively lower concentration. At 30° bTDC SoPI timing, less time 552 553 difference between pilot injection and the main injection dominated over superior in-554 cylinder conditions, which resulted in slightly inferior fuel-air mixing, leading to higher particulate number concentration. However at 40° bTDC SoPI timing, relatively inferior 555 dominated over longer time availability, leading 556 in-cylinder conditions to 557 inhomogeneous fuel-air mixing resulting in emission of higher number of particles. Due to presence of inferior in-cylinder conditions, soot nuclei formation increased, resulting 558 559 in higher particulate number concentration, however longer time availability affected 560 particulate size. Too advanced SoPI timing (40° bTDC) improved fuel-air pre-mixing and size of peak particulate number concentration decreased in comparison to intermediate 561 SoPI timing (35° bTDC). At 35° bTDC SoPI timing, particulate size distribution was 562 relatively wider in comparison to other SoPI timings. This indicated trade-off between 563 fuel-air pre-mixing time and in-cylinder conditions. In the experiment, 30° bTDC SoPI 564 565 showed maximum particle concentration (6x107 particles/cm³ exhaust gas) and 35° bTDC SoPI showed minimum particle concentration (3x10⁷ particles/ cm³ exhaust gas). 566 Particulate surface area-size distribution affects the toxicity of particulate because 567 higher surface area of particulate increases probability of surface adsorption of toxic 568

569 gaseous species and PAHs. Particle surface area was calculated by assuming them to be570 spherical.

571

$$dS = dN.(D_p)^2$$

Here dS is the area concentration of the size range with mean diameter D_p and dN is the 572 number concentration of particles with mean diameter D_p. Higher number concentration 573 of smaller particles results in higher surface area in comparison to surface area of lower 574 number of larger particles. Smaller particles have the ability to penetrate deeper in the 575 respiratory system, which enhances the possibility of them causing several diseases [40]. 576 Smaller particles also have longer retention time in the environment due to their lower 577 settling velocity. This increases their possibility to be inhaled in the human body. 578 579 Therefore smaller particles tend to become more hazardous for human health as opposed to larger particles. 580

From figure 8(b), it can be observed that particle surface area distribution decreased 581 with advancing SoMI timing. This trend was common at all SoPI timings. With 582 583 advancing SoPI timings, particulate surface area decreased continuously with trend slightly different from that of particle number-size distribution. Advancing SoPI timing 584 improved fuel-air pre-mixing, leading to lower particulate concentration. At too 585 advanced SoPI timing, particle number concentration increased slightly, however 586 particulate size distribution decreased. These two counter effects resulted in lower 587 particulate surface area. At too advanced SoPI timings (40° bTDC), wider particle 588 surface area-size distributions also showed the contribution of larger particles to the 589 total particulate surface area. This showed that contribution of larger particles ($D_p > 200$ 590 591 nm) to the total particulate surface area was almost equal to the contribution of small particles ($D_p < 200$ nm). Due to longer time availability for fuel-air premixing, variation 592 of SoMI timing was slightly less effective at advanced SoPI timings. Overall, the results 593 at different SoPI timings suggested that intermediate SoPI timing was suitable for 594

595 PCCI combustion because it resulted in larger particulates in lower number 596 concentration, which are less harmful to the human health.

597 Figure 9 (a) shows particle number-size distribution at varying EGR rates and SoMI598 timings.

599

Figure 9: (a) Number-size and (b) surface area-size distributions of particulate at

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varying EGR rates and SoMI timings

Similar to SoPI results, advancing SoMI timing resulted in lower particulate number 601 602 concentration however reduction at advanced SoMI timings was higher at 0 and 30% 603 EGR rates compared to 15% EGR rate. Figure 9(a) showed that the particle number concentration first decreased with increasing EGR rate (up to 15%) and then increased 604 drastically with further increasing EGR rate up to 30%. There were two factors 605 responsible for this observation. First was the shifting of combustion phasing, which 606 improved combustion efficiency leading to lower number of soot nuclei formation. Second 607 factor was the dilution effect, which reduced in-cylinder temperature and increased 608 609 particulate formation near the cylinder walls (due to presence of fuel-rich pockets formed during combustion quenching and spray impingement). When EGR rate 610 611 increased up to 15%, the first factor dominated, resulting in lesser particulate number 612 emissions. However at 30% EGR rate, second factor dominated, resulting in significantly higher particulate number emissions. With increasing EGR rate, peak of particle 613 number-size distribution also shifted towards larger particles. This was mainly due to 614 lower in-cylinder temperatures at higher EGR rate, which promoted condensation of 615 volatile organic species. These condensates were adsorbed on to the primary particulate 616 617 surface, resulting in larger particles. Figure 9(b) shows that the particulate surface area-size distribution followed similar trend as that of particulate number-size 618 distribution. With increasing EGR rate, particulate surface area increased due to 619 formation of larger particulate. At 30% EGR rate, peak of particulate surface area 620

significantly increased compared to 0 and 15% EGR rates. This was mainly due to
higher number concentrations of relatively smaller particles. Amongst all three EGR
conditions, 15% EGR rate was found to be most suitable for PCCI combustion mode
because of its lower particulate number as well as surface area distributions.

Overall analysis of particulate emitted from PCCI combustion mode was carried out in 625 terms of nucleation mode particles (NMP) ($D_p < 50$ nm) and accumulation mode particles 626 (AMP) (50 nm< D_p < 1000 nm) concentrations; total particle number (TPN) 627 concentration and count mean diameter (CMD) (Figure 10). These parameters were 628 629 calculated from particulate number-size distributions. Figure 10(a) shows the analysis of particulate emitted from PCCI combustion at different SoPI and SoMI timings. With 630 advanced SoMI timings, NMP concentration remained almost constant at 30° and 40° 631 bTDC SoMI timings, however it slightly decreased at 35° bTDC timing. This showed 632 633 that the formation of NMP was affected by two factors: (i) in-cylinder conditions, and (ii) fuel-air pre-mixing time. At too advanced or retarded SoPI timings, one factor always 634 635 dominated, resulting in higher NMP. At intermediate SoPI timing, trade-off among these two factors showed the effect of variations in SoMI timing, which increased the 636 637 fuel-air pre-mixing and resulted in lower NMP concentration. Amongst all three SoPI timings, 35° bTDC resulted in lowest NMP concentration. At all SoPI timings, NMP 638 concentration was > 1×10^8 particles/cm³ of exhaust gas, which was significantly lower 639 than HCCI combustion and conventional CI combustion modes [38]. With advanced 640 SoMI timing, AMP concentration slightly decreased due to improved fuel-air pre-mixing. 641 AMP concentration also followed similar trend as that of NMP. However AMP 642 concentration (~4x10⁸ particles/cm³ of exhaust gas) was higher than NMP concentration 643 (~1x10⁸ particles/cm³ of exhaust gas). 644

Figure 10: Number of Nucleation mode particles, number of accumulation mode 645 particles, total particulate number, and count mean diameter of particulate for varying 646 647 SoMI timings at different (a) SoPI timings and (b) EGR rates Figure 10(a) shows that 30 and 35° bTDC SoPI timings showed the highest TPN 648 concentration ($\sim 5 \times 10^8$ to 6×10^8 particles/cm³ of the exhaust gas) and the lowest TPN 649 concentration (~3x10⁸ to 4x10⁸ particles/cm³ of exhaust gas) respectively. For all SoPI 650 timings, advancing SoMI timings resulted in relatively lower TPN concentration. At 24° 651 bTDC SoMI timing, reduction in TPN concentration was slightly lower due to inferior 652 in-cylinder conditions. Advancing SoPI timing also resulted in lower TPN concentration, 653 however too advanced SoPI timing led to slightly higher TPN concentration due to 654 inferior fuel vaporization in presence of lower in-cylinder temperatures. Average size of 655 particulate emitted at different SoPI and SoMI timings were presented by CMD. CMD 656 showed the number averaged diameter of particulate. Results showed that particulate 657 emitted at 35° bTDC SoPI timing had the highest CMD and particles emitted from 30° 658 bTDC SoPI timing had the lowest CMD. At 12° SoMI timing, CMD of particulate at 659 different SoPI timings was almost same. This was attributed to longer time difference 660 661 between SoPI and SoMI timings, which decreased with advancing SoMI timings. At 35 and 40° SoPI timing, CMD increased with advancing SoMI timings, however CMD was 662 almost constant at 30° bTDC SoPI timing. CMD varied mainly due to variations in 663 particle number as well as particle size. 664

Figure 10(b) shows the variations in NMP, AMP and TPN concentrations, and CMD of particulate emitted from PCCI combustion at different SoMI timings and EGR rates. NMP concentration remained almost same at different EGR rates. With increasing EGR rates, AMP concentration increased due to reduction in peak cylinder temperature and chemical kinetics of fuel-air mixtures. These two factors promoted formation of higher number of soot nuclei as well as particulate agglomeration. At 15% EGR rate, AMP

concentration remained almost constant, however at 30% EGR rate, AMP concentration 671 increased drastically. At 15% EGR rate, particulate number concentration decreased 672 673 due to slightly improved combustion phasing. At 30% EGR rate, too retarded 674 combustion phasing resulted in emission of large number of particulate. TPN trends showed that 30% EGR rate resulted in maximum TPN concentration (~7x10⁸) 675 particles/cm3 of exhaust gas) and 15% EGR rate resulted in minimum total particle 676 concentration ($\sim 3x10^8$ particles/cm³ of exhaust gas). Advancement of SoMI timing led to 677 lower TPN concentration. Variations in CMD of particulate showed that 30% EGR rate 678 resulted in formation of larger particles compared to 0% and 15% EGR rates. Increasing 679 680 EGR rate enhanced condensation of volatile species due to lower in-cylinder temperatures. These condensates were adsorbed on to primary particulates, which 681 increased the particulate size, leading to higher CMD. 682

Particulate analysis showed that 35° bTDC SoPI timing was most suitable for PCCI combustion mode. At 35° bTDC SoPI timing, TPN concentration was lowest with the highest CMD, which reduced their potential harmful effects. Comparison of particulate emission characteristics at different EGR rates showed slight reduction in particulate number concentration at 15% EGR rate and significantly higher particulate number concentration at 30% EGR rate. Therefore 15% EGR rate was suitable for PCCI combustion.

690 3.5 Particulate Bound Trace Metals

For detailed particulate analysis, particulate samples were analyzed for trace metals. The experiments were carried out in two stages. In the first stage, effect of SoPI timings was investigated by analyzing three particulate samples collected at SoPI timings of 30, 35 and 40° bTDC. In the second stage, effect of EGR was investigated by analyzing three particulate samples collected at EGR rates of 0, 15 and 30%. During these experiments, all other parameters such as SoMI and FIP were maintained constant at 16° and 700

bar respectively. In trace metal analysis, total of 34 trace metals were detected in the particulate samples, however only 20 trace metals, which could be detected with <90% accuracy level are discussed here. These trace metals were further classified into five groups based on their origin, their health effects and for convenience of presentation (figure 11).

702 703

rates

Figure 11: Particulate bound trace metals at different (a) SoPI timings and (b) EGR

Figure 11 shows particulate bound trace metals emitted from the engine at different 704 SoPI timings and EGR rates during PCCI combustion mode. First group contained 705 706 traces of Al, Cu, Fe and Zn, which are harmful for human health due to their reactive 707 oxygen species (ROS) generation potential, and can lead to onset of cancer. Main source 708 of these trace metals are the wear debris of engine components. These wear debris are picked up by the lubricating oil, which is recirculated in an engine in order to reduce 709 friction between piston rings and cylinder liner interface. During combustion, pyrolysis 710 711 of lubricating oil also contributes to these trace metals in the particulate. Zinc containing compounds are commonly used as additives in lubricating oils and greases. 712 713 During combustion, these compounds undergo thermo-oxidative decomposition in 714 presence of oxygen to form zinc poly phosphate, which gets converted into ZnO and emitted as trace metal. At advanced SoPI timings, improved fuel-air mixing resulted in 715 716 lower particulate emissions with consequently lower trace metal content. Increasing EGR rate showed significant reduction in concentration of these trace metals in the 717 particulate. At higher EGR rate, lower in-cylinder temperatures reduced pyrolysis of 718 719 lubricating oil, leading to lower emissions of these trace metals, which is different from 720 HCCI combustion trace metals emission characteristics [28]. Results showed that the concentration of Al and Fe traces decreased with advancing SoPI timings, however Cu 721 and Zn trace concentrations slightly increased at 35° bTDC SoPI timing. In this group, 722

Al concentration was relatively higher (~8 to 10 ppm/mg of PM) compared to other trace 723 metals. Second group of trace metals included Ca, K, Na and Mg. Pyrolysis of 724 725 lubricating oil was the main source of these metals. These trace metals are a part of different organo-metallic additives added to the lubricating oil in order to improve its 726 727 lubricity, corrosion resistance, etc. Concentrations of these trace metals were slightly higher in PCCI combustion mode. These trace metals do not affect human health 728 therefore these trace metals were not much discussed in previous studies [28, 41]. 729 Advancing SoPI timings didn't show significant variation in concentration of these trace 730 metals. Results showed that trace concentrations of Ca, Na and Mg decreased with 731 increasing EGR rate since lower in-cylinder temperatures reduced pyrolysis of 732 733 lubricating oil. The third group of trace metals included Ni, Cr, Cd and As, which primarily originate from wear of metallic engine components and lubricating oil 734 additives. These metals are not harmful in their pure form however they easily combine 735 with other species to form highly toxic compounds. Lower concentration of Ni, Cd and As 736 737 was due to relatively lower in-cylinder temperature during PCCI combustion mode. Nickel is used as an additive in the lubricating oil in very small concentration as Nickel 738 ethoxy-ethyl-xanthate for improving lubrication quality. Upon combustion, these 739 740 compounds dissociate to release nickel, which reacts with sulphur and forms a carcinogenic compound NiS [42]. Concentration of Ni emitted from PCCI engine was 741 significantly lower compared to HCCI engine, which was mainly due to lower particulate 742 emission (Figure 8) [28]. In the experiments, Cr was found to be in relatively higher 743 744 concentration and its trace concentration decreased with advanced SoPI timing and 745 increasing EGR rate. This trend is different from gasoline fuelled HCCI combustion in which Cr concentration slightly increased with increasing EGR rate [41]. Fourth group 746 of trace metals included Pb, Mo, Sr and Ba, which primarily originate from fuel, 747 lubricating oil and sometimes from wear of engine components such as gaskets, piston 748

rings, etc. Pb, Mo, Sr and Ba are also harmful for human health. These trace metals 749 didn't show any specific trend in variation with SoPI timings. Pb, Mo and Sr 750 751 concentrations decreased with increasing EGR rate. Lower in-cylinder temperatures at 752 higher EGR rates were the main reason for this trend, which reduced the deterioration 753 of softer engine components such as gaskets and seals. However Pb, Sr and Ba were lowest for 15% EGR rate. Last group of trace metals included Mn, Bi, In and V, which 754 are generally used in engine components to enhance their properties. Therefore wear of 755 engine components was the main source of these metal traces. Concentration of these 756 757 trace metals were found to be very low, which didn't show any specific trend at different 758 SoPI timing and EGR rate.

Comparison of trace metals emitted from PCCI combustion and HCCI combustion shows one important finding that concentration of harmful trace metals were significantly lower in PCCI combustion mode [28]. This was attributed to lower particulate emissions from PCCI combustion mode. Therefore this study clearly indicates that optimized PCCI combustion is beneficial for particulate reduction compared to HCCI combustion.

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765 3.5 Statistical Analysis

To compare different split injection stratgeies and EGR rates, statistical analysis of PM mass and NOx emissions was plotted. This analysis gave a direct comparison of effectiveness of combustion at different fuel injection strategies and EGR rates. Height of rectangle showed particulate mass and width of the rectangle represented NOx emission. Area of the rectangle represented the combined emission of PM and NOx. Overall objective of this study was to reduce the area under the curve.

Figure 12: NOx-PM mass analysis at varying (a) SoPI timings and (b) EGR rates in

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PCCI combustion mode

Figure 12 (a) shows the variation of brake specific NOx (BSNOx) with PM mass 775 emissions at different SoMI and SoPI timings. In all cases, it was observed that 776 777 advancing SoMI timings resulted in higher NOx but lower PM emissions. This was attributed to longer time availability for fuel-air mixing, which resulted in superior 778 combustion and led to slightly higher NOx emission. For a particular SoMI timing, 779 advancement in SoPI timing from 30 to 35° bTDC resulted in simultaneous reduction in 780 PM and NOx. However further advancement in SoPI timing led to lower PM (due to 781 more time available for fuel-air pre-mixing) but higher NOx emissions. Due to slightly 782 783 inferior cylinder conditions, performance and combustion also degraded at 40° bTDC compared to 35° bTDC. PM and NOx emission showed an interesting behavior with the 784 785 EGR rate (Figure 12(b)). An increment in EGR rate from 0 to 15% simultaneously reduced NOx and PM emissions. NOx emissions reduced primarily due to lower in-786 cylinder temperatures. An increase in EGR rate led to slower chemical kinetics of fuel-787 air mixtures, which resulted in slightly retarded combustion phasing. Retarded 788 789 combustion phasing increased overall combustion duration, which provided sufficient time for soot oxidation, led to relatively lower PM emission. However 30% EGR led to 790 791 very low combustion temperature, which reduced NOx emissions significantly. However 792 incomplete combustion resulted in drastically higher PM emissions. Poor engine performance and higher PM emission at 30% EGR made it unsuitable for PCCI 793 combustion mode. Therefore, 15% EGR rate and 35° bTDC SoPI timing were found to be 794 the most suitable conditions for PCCI combustion mode in a medium-duty diesel engine. 795

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797 <u>Conclusions</u>

798 This experimental study was carried out to investigate suitable split injection 799 parameters and EGR rate for optimized PCCI combustion. The experiments were 800 carried out at different SoMI timings (12 to 24° bTDC), SoPI timings (30 to 40° bTDC)

801 and EGR rates (0, 15 and 30%). During the experiment, FIP was maintained constant at 700 bar. Results showed that advancing SoMI and SoPI timings improved PCCI 802 803 combustion, but too advanced SoPI timings resulted in slightly inferior performance and emission characteristics. Advancing SoPI from 30 to 35° bTDC improved chemical 804 kinetics of fuel-air mixture and led to slightly higher P_{max} and highest HRR. At 40° SoPI 805 timing, combustion degraded slightly due to inferior combustion chamber conditions. 806 SoPI timing didn't show any significant effect of the SoC and combustion phasing. 807 Advancing SoPI timing reduced knocking and resulted in lower knock peak and 808 combustion noise. BTE improved slightly at SoPI timing of 35° bTDC however it 809 drastically reduced at SoPI timing of 40° bTDC. EGT also showed that intermediate 810 811 SoPI timing was suitable for PCCI combustion. NOx, and smoke opacity were slightly lower at SoPI timing of 35° bTDC. Particulate number concentration was the minimum 812 813 and average particulate size was the maximum at this condition as well. Particulate bound trace metals didn't show any significant variation with changing SoPI timings. 814 815 Statistical analysis showed that advanced SoPI timing reduced PM mass and NOx emissions simultaneously, however too advanced SoPI timing led to slightly higher NOx 816 817 emissions. Increasing EGR rate effectively controlled the HRR during PCCI combustion 818 mode, but very high EGR rate resulted in ultra-dilution of the combustible charge. This led to very low peak in-cylinder temperature, resulting in very low BTE and higher HC 819 and CO emissions. Increasing EGR rate reduced the knocking and combustion noise 820 though. With higher EGR rate, NOx emission decreased but PM mass emission 821 822 increased significantly. Trace metal analysis revealed that PCCI combustion emitted 823 relatively lower trace metals compared to HCCI combustion and concentration of most of the reported trace metals decreased with increasing EGR rate. Overall effectiveness of 824 EGR on PCCI combustion mode was indicated by the statistical analysis. With 825 increasing EGR rate, NOx and PM mass emission decreased simultaneously however 826

too high an EGR rate led to significantly higher PM mass emission. Therefore, it can be
concluded that optimum SoI timings and EGR rate can effectively control and enhance
engine performance and reduce emissions further in the PCCI combustion mode.

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1- Single cylinder research engine, 2- Transient dynamometer, 3- Dynamometer controller, 4- Coolant
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8- Air-flow rate measurement system, 9- Combustion data acquisition system, 10- ECU interface system, 11970
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Figure 1: Schematic of the experimental setup



976 Figure 2: Variations in cylinder pressure and HRR w.r.t. crank angle at different SoPI

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and SoMI timings



980 Figure 3: Variation in cylinder pressure and HRR w.r.t. crank angle for different SoMI

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timings and EGR rates



985 Figure 4: SoC, combustion phasing and combustion duration w.r.t. SoMI timings at

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different (a) SoPI timings and (b) EGR rates





991 Figure 5: Variation in knock integral, knock peak and combustion noise w.r.t. SoMI

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timings at different (a) SoPI timings and (b) EGR rates



995 Figure 6: Variations in BTE, BSFC and EGT w.r.t. SoMI timings at different (a) SoPI

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timings and (b) EGR rates



999 Figure 7: Variations in mass emissions of CO, HC, NOx and smoke opacity w.r.t. SoMI

timings at different (a) SoPI timings and (b) EGR rates



1003 Figure 8: (a) Number-size and (b) Surface area-size distributions of particulate at

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varying SoPI and SoMI timings, and 15% EGR rate





varying EGR rates and SoMI timings



Figure 10: Number of Nucleation mode particles, number of accumulation mode 1011 1012 particles, total particulate number, and count mean diameter of particulate for varying 1013 SoMI timings at different (a) SoPI timings and (b) EGR rates



1016 Figure 11: Particulate bound trace metals at different (a) SoPI timings and (b) EGR

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rates



Engine Parameters	Specifications
Engine make/ model	AVL/ 5402
Number of cylinder/ s	1
Cylinder bore/ stroke	85 mm/ 90 mm
Swept volume	510.7 cc
Compression ratio	17.5
Inlet ports	Tangential & swirl ports
Maximum power	6.25 kW
Rated speed	4200 rpm
High pressure system	Common rail direct injection BOSCH CP4.1
Engine management system	AVL-RPEMS + BOSCH ETK7
Valves per cylinder	4 (2 inlet, 2 exhaust)
Valve train type	DOHC cam follower
Liner type/ base	Wet

Table 1: Technical specifications of the test engine

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