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**Parametric investigation of pre-injection on the combustion, knocking and emissions behaviour of a large marine four-stroke dual-fuel engine**

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21

22 **Nomenclature**

23

24 DF: Dual-fuel

25 CA: Crank Angle

26 TDC: Top Dead Center

27 BTDC: Before Top Dead Center

28 ATDC: After Top Dead Center

29 IMEP: Indicated Mean Effective Pressure

30 HRR: Heat Release Rate

31 THC : Total Hydrocarbon

32 NO<sub>x</sub> : Nitrogen Oxide

33 1-D : One-Dimensional

34 3-D: Three-Dimensional

35 CFD: Computational Fluid Dynamics

36 KI: Knock Index

37 MP: Monitoring Points

38 LNG: Liquefied Natural Gas

39 IVC: Intake Valve Closing

40 EVO: Exhaust Valve Opening

41 SOI: Start of Injection

42 SOPI : Start of Pre-Injection

43 PMR: Pre-Injection Mass Ratio

44 PMI: Pre-Injection and Main Injection Interval

45 SOMI: Start of Main Injection

46 MMR: Main Injection Mass Ratio

47 PFP: Peak Firing Pressure

48 PFPCA: The Crank Angle of Peak Firing Pressure

49 THR: Total Heat Release

- 50 DI : Direct Injection
- 51 FAT: Factory Acceptance Test
- 52 ASI: After Start of Injection
- 53 AMR: Adaptive Mech Refinement
- 54 IMO: International Maritime Organization

55

56 **Abstract**

57

58 This study aims at the parametric investigation of a large marine four-stroke dual-fuel engine in  
59 order to identify the pre-injection effects on the engine combustion, knocking and emissions parameters.  
60 A model was employed that was developed by integrating a 1-D engine model in AVL-BOOST and a 3-D  
61 CFD model in CONVERGE. The MAN 51/60DF marine engine is modelled and the simulation results  
62 were validated against experimental data. Subsequently, parametric runs for various pre-injection timings  
63 and mass ratios are performed and the simulation results are analysed and discussed. The derived in-  
64 cylinder pressure oscillations at determined points are employed to calculate the knock index (KI), which  
65 was used as an evaluation indicator for the knocking intensity. A number of pre-injection strategies with  
66 varying timing and fuel mass ratios are studied. This study results reveal that a lower knock trend and  
67 NO<sub>x</sub> emissions can be achieved by early pre-injection timing and increasing pre-injection fuel mass ratio.  
68 In addition, the medium pre-injection interval increases the engine IMEP while reducing the NO<sub>x</sub> and  
69 total hydrocarbon emissions. Larger pre-injection mass ratio reduce the KI and NO<sub>x</sub> emissions, but  
70 reduces IMEP and causes the wetted-wall phenomenon. Besides, the excessive pre-injection intervals and  
71 pre-injection mass ratio result in a change in combustion mode from the conventional diesel compression  
72 ignition mode to a two-stage auto-ignition mode. This study provides a better understanding of the  
73 underlying interactions of involved parameters and proposes pre-injection solutions to improve the engine  
74 performance, emissions and knocking behaviour.

75 *Keywords:* Large marine DF engine; Pre-injection Strategies; Knocking; Combustion; Emissions

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## 79 1. Introduction

80

81 The main power machinery is the diesel engine in the marine field, due to the advantages of high  
82 power, high efficiency, low energy consumption and high reliability [1]. At the same time, marine  
83 engines emit a wide variety of pollutants that have important impacts on health and climate change [2].  
84 Policies and regulations to reduce nitrogen oxide ( $\text{NO}_x$ ) emissions are strict, especially those rules aiming  
85 at exhaust emissions restriction of marine engines, which are major  $\text{NO}_x$  emissions sources [3]. In  
86 particular, the International Maritime Organization (IMO) has established specific emissions limitations  
87 for marine diesel  $\text{NO}_x$  pollutants [4]. IMO Tier III standard drastically limits the  $\text{NO}_x$  emissions equal to  
88 80 % of the Tier I standard [5]. Natural gas, which is the most used fossil fuel and the premium fuel of the  
89 twenty-first century, is desirable for various utilizations [6]. The use of liquefied natural gas (LNG) for  
90 ship propulsion reduces  $\text{NO}_x$ ,  $\text{SO}_x$  emissions as its higher H/C ratio characteristic compared with diesel  
91 or heavy fuel oils [7]. The natural gas has a more attractive price advantage when taking the market  
92 fluctuations and fuel prices into account. Compared to other fossil fuels, natural gas is being developed at  
93 an ever-increasing rate in the world due to its environmental benefits [8]. Domestic natural gas supplies  
94 are increasing, and natural gas prices have remained lower than oil prices over the past decade [9].  
95 Natural gas-diesel dual-fuel (DF) engines produce lower  $\text{NO}_x$  emissions when compared to conventional  
96 diesel engines [10]. The dual-fuel engine with low-pressure direct injection (DI) mode is a classical  
97 application mode, which retains the structure of the traditional engine to the greatest extent [11].

98 To improve the performance of dual-fuel engines, reduce emissions, and optimize the in-cylinder  
99 combustion process, the researchers have carried out relevant experimental and simulation studies [12-  
100 17]. The natural gas exhibits greater resistance to knocking due to its higher octane numbers (up to 120)  
101 and auto-ignition temperatures [18, 19]. However, the complex chemical kinetic characteristics of dual-  
102 fuel and the unique physical and chemical characteristics of natural gas lead to poor engine combustion  
103 stability, knock and other problems [20-23]. The experimental and simulation methods were adopted by  
104 many researchers, which are used to improve the performance of dual-fuel engines, reduce emissions, and  
105 optimize the in-cylinder combustion process [24]. Stoumpos et al. [25] investigated the effect of engine  
106 parameters on the performance of a large marine dual-fuel engine model by using one-dimensional (1-D)  
107 GT-Power. Considering the injection methods of two different fuels, the DF model was further

108 developed. This study provided a solution for reducing CO<sub>2</sub> and NO<sub>x</sub> emissions when considering engine  
109 operating limits simultaneously. Yousefi et al. [26] studied the effect of diesel injection timing dual-fuel  
110 combustion at low load through an experimental and numerical research. The results showed that the NO<sub>x</sub>  
111 emissions first increased and then decreased, and the coefficient of variation of IMEP decreased with the  
112 advance of injection timing. Liu et al. [27] studied the ignition characteristics and pressure oscillation of a  
113 low-speed marine low-pressure DI natural gas dual-fuel engines. The numerical research showed that the  
114 amplitude of pressure oscillation increased with the later injection timing of the pilot fuel. Liu et al. [28]  
115 studied injection strategies on a low-speed marine low-pressure DI natural gas DF engines with a pre-  
116 chamber. Three factors were considered, including variable absolute injection timing, variable pilot fuel  
117 injection, and variable gas fuel injection. The results showed that the advanced gas fuel injection and  
118 retarded pilot fuel injection timings led to partially premixed gas burn, and further advanced or retarded  
119 timings resulted in a more partially premixed gas burn. In addition, the effects of pilot fuel mass and  
120 equivalence ratio on ignition / extinction and pressure oscillation were investigated by Liu et al. [29].  
121 Yuan et al. [30] investigated the miller cycle and pre-injection on a low-speed marine high-pressure DI  
122 natural gas DF engines numerically. The results showed that, compared with the pre-injection mass ratio,  
123 the injection interval had little effect on the pressure oscillation, but the excessive injection interval  
124 affected the combustion stage. Valladolid et al. [31] conducted a numerical study on the effect of diesel  
125 pilot distribution on the ignition process of the DF medium-speed marine engine. They found that, the  
126 diesel injection pressure had a larger impact on NO<sub>x</sub> for early injection timings than that for late injection  
127 timings. Xu et al. [32] experimentally studied the pre-injection strategy for pilot diesel compression  
128 ignition natural gas engines. The experimental results showed that the pre-injection timing reduced the  
129 ignition intensity which decreased the burning rate of the gas mixture and lowered NO<sub>x</sub> emissions. Zhao  
130 et al. [33] experimentally studied the pre-injection strategy of a diesel/natural-gas DF engine, which was  
131 modified from a six-cylinder direct injection common rail diesel engine. The results showed that the  
132 ignition phase was controlled by the main injection, which avoided the worsen combustion stability  
133 caused by the inconsistent ignition phase.

134 Based on the briefly reviewed literature above, it is revealed that the injection strategy has great  
135 potential for reducing the knock tendency, improving engine performance, improving fuel economy, and  
136 reducing emissions [30, 32]. However, fewer studies have been conducted on the laws of influence of pre-

137 injection parameters on knock, combustion and emissions, and methods to optimize pre-injection  
138 parameters, especially in the field of marine medium speed large-bore DF engine [31, 34]. Due to the  
139 large size of marine DF engines, it is difficult to carry out relevant experiments [27, 35, 36]. The  
140 numerical simulations have been widely accepted as the best way and partial alternative to the research of  
141 large marine engines [3, 37]. DF engines have a wider lambda window and lower propensity to knock at  
142 low loads, but with low thermal efficiency, and high levels of NO<sub>x</sub> and total hydrocarbon emissions.  
143 Therefore, the objective of this work is to understand the effect of the pre-injection strategy on the knock,  
144 combustion and emissions in a large marine medium-speed DF engine at low load.

145 In this study, the process of in-cylinder combustion and pressure development of a DF engine at low  
146 load was studied by using a three-dimensional (3-D) numerical simulation method [38]. The pre-injection  
147 strategy was simulated for combustion stability and knock of a large marine DF engine by commercial  
148 CONVERGE code. The novel contributions of this work include: Firstly, the effect of the pre-injection  
149 strategy on the combustion mode was elaborated. Further, the conditions and criteria for the occurrence of  
150 knock phenomena were revealed. Moreover, the knock index was defined with reference to the gasoline  
151 engine and was used as an indicator for the evaluation of the pre-injection strategy. The effects of pre-  
152 injection timing and pre-injection quantity on knock, combustion and emissions were analyzed of a large  
153 marine DF engine at low load, which provided an important theoretical basis for the pre-injection strategy,  
154 improving the actual engine combustion stability, avoiding the phenomenon of knock, and improving  
155 engine combustion and emissions characteristics.

156

## 157 **2. Modeling methodology**

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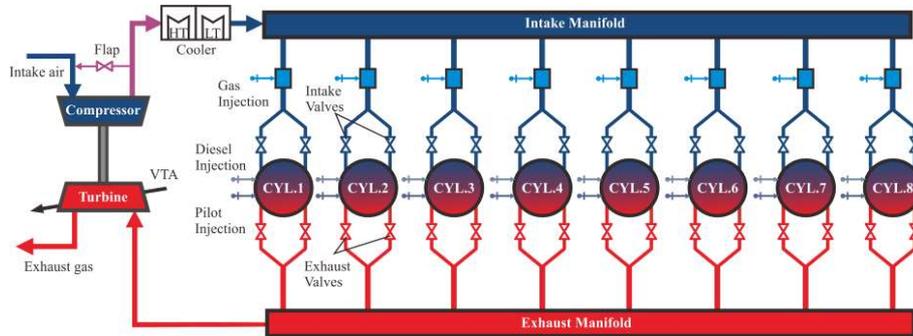
### 159 **2.1. Investigated engine**

160

161 The MAN 8L51/60 DF engine, which was a four-stroke, variable injection timing, turbocharged and  
162 intercooled DF engine, was used for the present study. The engine consists of eight cylinders placed in-  
163 line [39]. This type of engine is widely used due to its high power output, fuel flexibility, low emission  
164 rates, high efficiency and reliability. The natural gas is injected at each cylinder inlet port (upstream the  
165 intake valves) during the engine intake stroke. The pilot diesel fuel is injected directly into cylinders to

166 ignite the gas mixture before top dead center. The engine details are reported in the manufacturer project  
 167 guide [39] and factory acceptance test (FAT). The engine layout and components are presented in Fig. 1  
 168 [39]. The main particulars are listed in Table 1 [39].

169



170

Fig. 1. Engine layout and components [39]

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173

Table 1 MAN 8L51/60DF test engine specifications

Terms	Unit	Value
Cylinder number	[-]	8
Bore	[mm]	510
Stroke	[mm]	600
Compression ratio	[-]	13.3
Rated power	[kW]	8000
Rated speed	[r/min]	514
Mean effective pressure	[bar]	19.1
BSFC (Diesel model)	[g/kW·h]	189.1
BSEC (Gas model)	[kJ/kW·h]	7998
Turbocharger units	[-]	1
Fire order	[-]	1-4-7-6-8-5-2-3

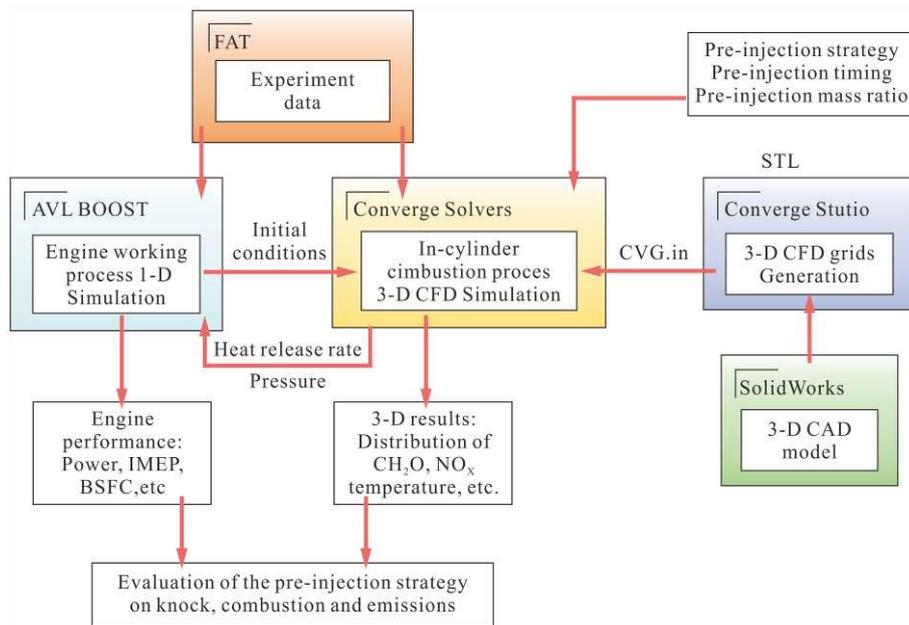
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175 **2.2. Model set-up and calibration**

176

177 In this paper, the combustion chamber geometry was modeled by using SolidWorks software. The  
 178 Converge Studio was used to arrange the boundary, set calculation model and change calculation  
 179 conditions. The CVG.in format data was the required files for Converge Solvers to calculate the  
 180 combustion. The simulation working process coupled with 3-D calculation and 1-D coupling calculation  
 181 is presented in Fig. 2. As can be seen from Fig. 2., the initial conditions of the 3-D model were provided  
 182 by the 1-D model and the 1-D model was calibrated by the FAT [40].

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Fig. 2. Process of 3-D calculation and 1-D coupling calculation

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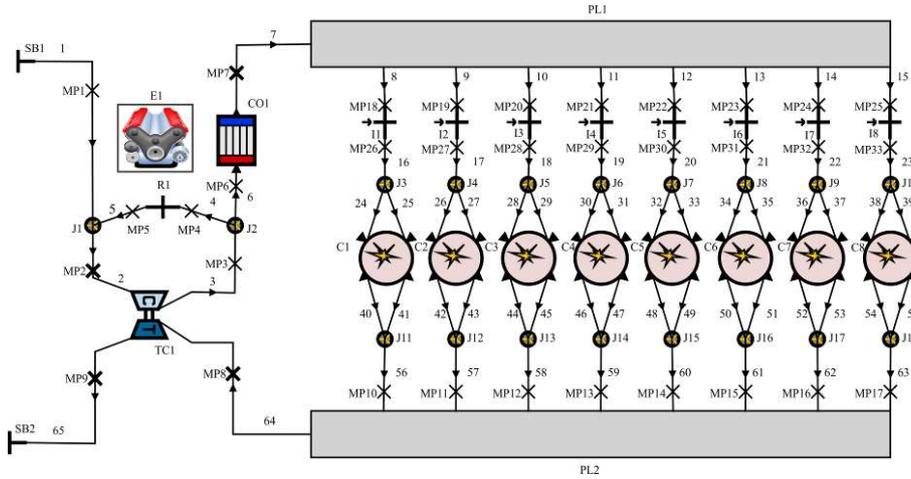
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### 187 2.2.2. 1-D simulation model calibration

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189 In this study, the boundary conditions and initial conditions were provided by using AVL-BOOST  
 190 [41], and in-cylinder combustion was calculated by using CONVERGE code [42]. The AVL-BOOST is  
 191 widely used in 1-D simulation for engine modeling and analysis [41]. The DF engine mode in AVL-  
 192 BOOST environment is presented in Fig. 3 [12]. The engine modeling and calibration were omitted here  
 193 and the general method can be found in our previous works [12, 43]. The validation results of the primary  
 194 parameters of DF engine model in the gas model are reported in Table 2 and Fig. 4 [12]. The parameters  
 195 in Fig. 4 were normalized based on 75% load.

196

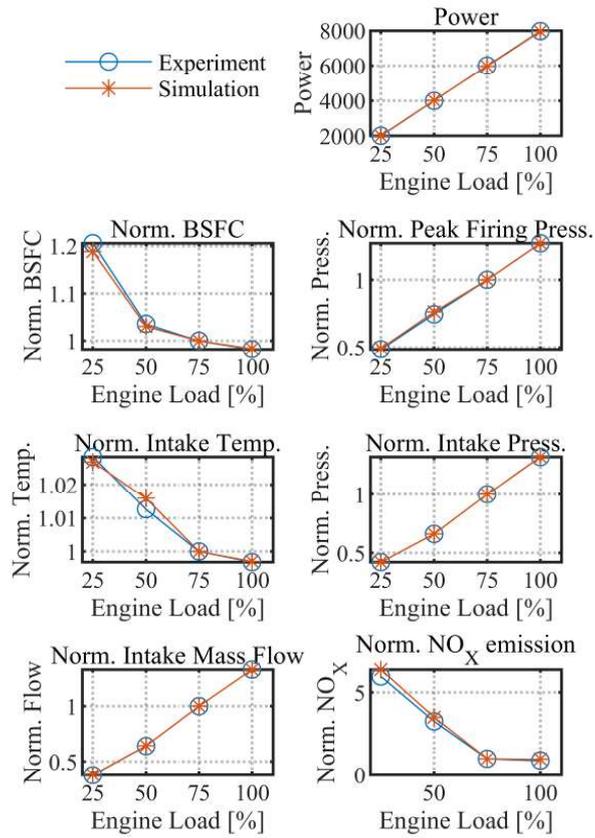


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Fig. 3. Dual-fuel engine mode in AVL-BOOST environment [12]

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200

201

Fig. 4. Validation results of primary parameter of model [12]

202

Table 2 Validation results of primary parameter of model [12]

Engine Load [%]	100	75	50	25
Mode	Gas Mode Error (%)			
Power [kW]	0.12	0.14	-0.09	0.38
BSFC [g/kW·h]	-0.09	-0.11	0.13	-0.34
Peak Firing Pressure [bar]	-1.81	-1.72	0.44	0.51
Intake Manifold Temperature [K]	-0.99	-0.64	0.34	-2.00
Intake Manifold Pressure [bar]	-0.04	-0.24	-0.12	-0.11
Intake Manifold Mass Flow [kg/h]	-0.12	-0.22	0.16	0.67
Exhaust Manifold Temperature [K]	-1.98	0.27	0.10	2.79
Exhaust Manifold Pressure [bar]	1.28	2.59	2.23	-0.62
Exhaust Manifold Mass Flow [kg/h]	-0.16	0.14	-0.09	0.38
NO <sub>x</sub> Emissions [g/kW·h]	1.59	-2.43	-1.96	1.98

204

205 **2.2.3. 3-D simulation model calibration**

206

207 In the CFD model, the marine engine numerical simulation also is based upon continuity,  
 208 momentum and energy conservation laws [42, 44]. The compressible equations for mass transport,  
 209 momentum transport and energy are given by Eqs. (1)-(3).

$$210 \quad \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = S \quad (1)$$

$$211 \quad \frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} + S_i \quad (2)$$

$$212 \quad \frac{\partial \rho e}{\partial t} + \frac{\partial u_j \rho e}{\partial x_j} = -P \frac{\partial u_j}{\partial x_j} + \sigma_{ij} \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j} \left( K \frac{\partial T}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left( \rho D \sum_m h_m \frac{\partial Y_m}{\partial x_j} \right) + S \quad (3)$$

213 In the above equations,  $u$  is velocity,  $\rho$  is density,  $S$  is the source term,  $P$  is pressure,  $T$  is  
 214 temperature,  $Y_m$  is the mass fraction of species  $m$ ,  $D$  is the mass diffusion coefficient,  $e$  is the specific  
 215 internal energy,  $K$  is the conductivity,  $h$  is the species enthalpy and  $\sigma_{ij}$  is the stress tensor [45].

216 In addition, each submodel needed to be determined, such as the turbulence model, combustion  
 217 model, spray model, etc [46]. The DF engines with two different property fuels are complicated not only  
 218 fluid flow, but also chemical reactions as well as heat and mass transfer. The suitable selection of models  
 219 was required to simulate the dual-fuel engine. The Blob injection model [47] was implemented to  
 220 simulate Liquid injection. The KH-RT model was applied to the simulation of spray breakup [48]. The  
 221 Frossling model [49] was used as an Evaporation model. The O'Rourke and Amsden model [50] was used  
 222 to calculate the wall heat transfer. Numerical simulation of RNG  $k-\epsilon$  two-equation equation model  
 223 coupled with a detailed chemical reaction had shown excellent simulation results in different types of  
 224 fuels and engines [46, 51-55]. The various reaction mechanisms can be adapted in SAGE combustion  
 225 model with a fast calculation [56]. As described by Turns [44], the mechanism of the multi-step chemical  
 226 reaction can be described as Eqs. (4).

$$227 \quad \sum_{m=1}^{M_{tot}} \nu'_{m,r} \chi_m \Leftrightarrow \sum_{m=1}^{M_{tot}} \nu''_{m,r} \chi_m \quad r = 1, 2, \dots, R_{tot} \quad (4)$$

228 where the  $\nu'_{m,r}$  and  $\nu''_{m,r}$  are the stoichiometric coefficients for the reactants and products,  
 229 respectively, for species  $m$  and reaction  $r$ ; The  $R_{tot}$  represents the total number of the reactions; And  
 230 the  $\chi_m$  means the chemical symbol for species  $m$ .

231 The  $\dot{\omega}_m$  represents the net production rate of species  $m$  and it can be described as Eqs. (5).

$$232 \quad \dot{\omega}_m = \sum_{r=1}^{R_{tot}} \nu_{m,r} q_r \quad (m = 1, 2, \dots, M_{tot}) \quad (5)$$

233 where the  $M_{tot}$  is the total number of species.

234 The rate-of-progress parameter  $q_r$  for the  $r^{\text{th}}$  reaction is given by Eqs. (6).

$$235 \quad q_r = k_{fr} \prod_{m=1}^{M_{tot}} [X_m]^{\nu'_{m,r}} - k_{rr} \prod_{m=1}^{M_{tot}} [X_m]^{\nu''_{m,r}} \quad (6)$$

236 where the  $[X_m]$  is the molar concentration of species  $m$ . The  $k_{fr}$  and  $k_{rr}$  are the forward and  
 237 reverse rate coefficients for reaction  $r$  respectively.

238 With the above equation, the governing equation for mass is given by Eqs. (7).

$$239 \quad \frac{d[X_m]}{dt} = \dot{\omega}_m \quad (7)$$

240 The governing equation for energy is given by Eqs. (8).

$$241 \quad \frac{dT}{dt} = \frac{V \frac{dP}{dt} - \sum_m (\bar{h}_m \dot{\omega}_m)}{\sum_m (X_m \bar{c}_{p,m})} \quad (8)$$

242 where the  $\bar{h}_m$  and  $\bar{c}_{p,m}$  are the molar specific enthalpy and molar constant-pressure specific heat of  
 243 species  $m$ , respectively. The  $V$ ,  $P$  and  $T$  are the volume, pressure and temperature, respectively. The  
 244 above equations are solved at each computational time-step and the species are updated appropriately.

245 In order to obtain a more accurate model, the spray model was calibrated in this paper. The  
 246 experimental data for calibration were obtained from Sandia National Laboratories [57, 58]. Sandia  
 247 National Laboratories performed the high-fidelity parameter measurements of spray penetration, liquid  
 248 length, vapor penetration, etc. in a constant-volume combustion vessel [57, 58]. The parameters of  
 249 ambient and fuel injector conditions for calibration are listed in Table 3. Detailed experimental data can  
 250 be found in the literature [58]

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Table 3 Ambient and fuel injector conditions [58]

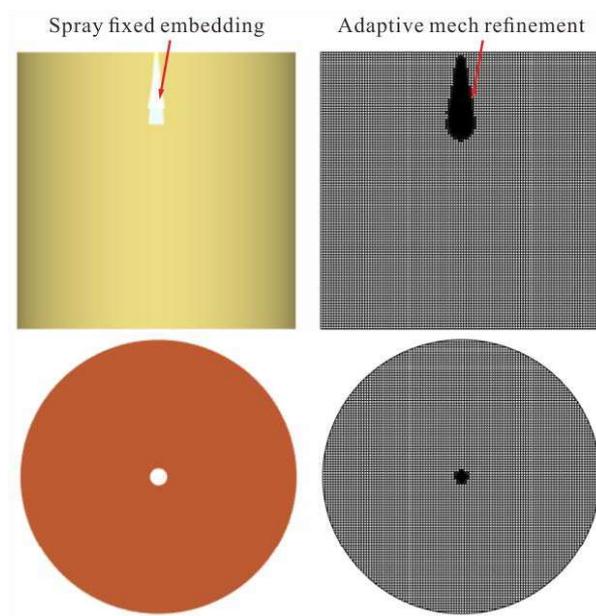
Terms	Unit	Value
Fuel type	[-]	<i>n</i> -heptane
Ambient temperature	[K]	1000
Ambient density	[kg/m <sup>3</sup> ]	14.8
Injection pressure	[MPa]	150
Fuel temperature	[K]	373
Nozzle diameter	[mm]	0.1
Injection duration	[ms]	6.8
Total mass injected	[mg]	17.8

253

254 The model used for calibration with the computational grid is presented in Fig. 5. As shown in Fig. 5,  
 255 spray fixed embedding and adaptive mech refinement (AMR) were used for the numerical simulation.  
 256 The diameter of the model is 108 mm and the height is 108 mm. The vaporizing diesel spray of  
 257 experiments and simulation are presented in Fig. 6. The experiments (instantaneous) was the

258 instantaneous measurements of vaporizing diesel spray by Rayleigh imaging. The experiments (mean)  
 259 was the mean behavior of the diesel spray which was computed from the dataset. It can be seen from the  
 260 Fig. 6 that the simulated penetration is almost consistent with the measured penetration, which shows the  
 261 accuracy of the spray model setting. Fig. 7 shows the comparison of vapor penetration. It can be seen  
 262 from the Fig. 7 that the simulation result at 0.8 ms is slightly smaller than the experiment. This is due to  
 263 the limitation of the larger grid and the RNG  $k-\epsilon$  model, resulting in the inability to capture vapor  
 264 penetration well [57]. Where the ASI is after start of injection.

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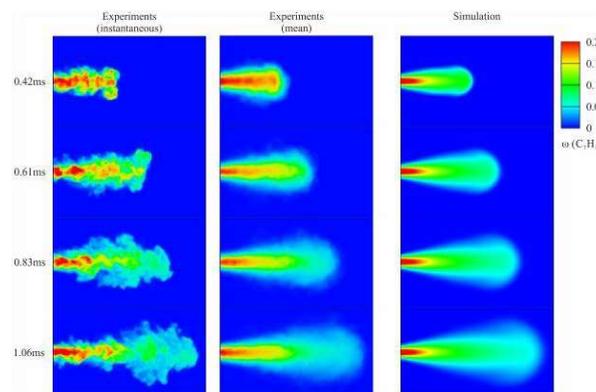


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Fig. 5. Model and grid for diesel spray simulation

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Fig. 6. Mixture fraction distributions

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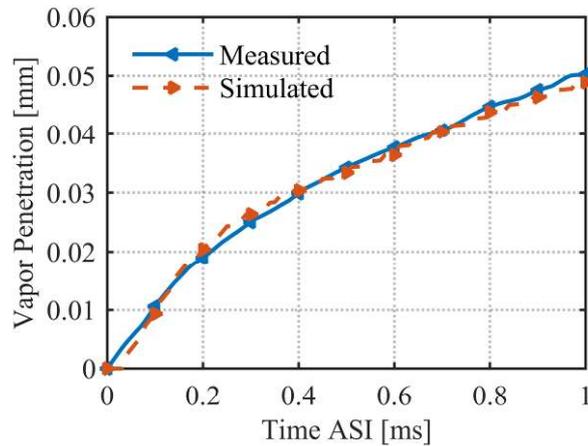


Fig. 7. Comparison of vapor penetration

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275 In DF numerical studies, the methane and n-heptane are commonly used as alternative fuels for  
 276 natural gas and diesel due to its similar physicochemical properties [29, 53]. The Extended Zeldovich  
 277 NO<sub>x</sub> mechanism was applied to simulate the production of NO<sub>x</sub> [59]. The DF mechanisms which were  
 278 developed by Rahimi, et al. [60] were obtained by merging n-heptane mechanisms and methane  
 279 mechanisms. This combustion mechanism was widely used in the combustion of DF engines and made it  
 280 possible to calculate cylinder pressure and NO<sub>x</sub> emissions more accurately[28, 29, 61]. The selected  
 281 mathematical models and chemical mechanisms are listed in Table 4. The combustion chamber geometry  
 282 was modeled by using SolidWorks software and exported as an STL file, then imported into the  
 283 CONVERGE software for boundary division [42]. The layout of the pilot injector with four holes in  
 284 CONVERGE environment is presented in Fig. 8. As it is shown, the pilot injector is not located in the  
 285 center of the cylinder, so the sector model cannot be used [39].

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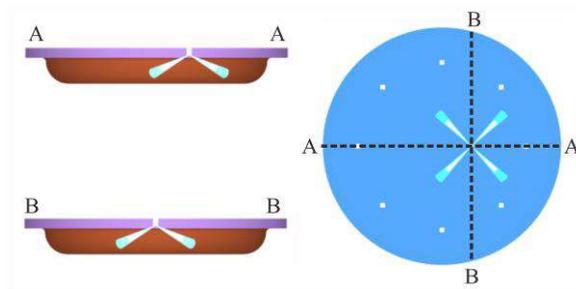
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Table 4 Mathematical models and chemical mechanisms

Model	Setting
Turbulence	RNG k-ε model [49]
Spray breakup	KH-RT model [48]
Combustion	SAGE model [56]
NO <sub>x</sub> formation	Extended Zeldovich model [59]
Reaction kinetics	Dual-fuel mechanism (GRI-Mech 3.0 and n-heptane) [60]

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Fig. 8. The layout of pilot injector in CONVERGE environment

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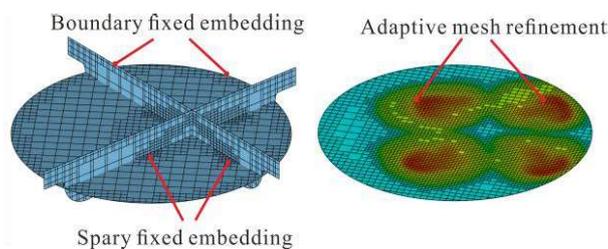
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The grid control strategy in CONVERGE code is presented in Fig. 9. As it is shown, the grid control strategy includes a base value grid, adaptive mesh refinement, fixed embedding and grid scaling [42]. In this paper, the max embedding level and sub grid criterion of velocity adaptive mesh refinement were set to 2 layers and 2.0 m/s respectively. The max embedding level and sub grid criterion of temperature adaptive mesh refinement were set to 2 layers and 5.0 K respectively. The injection fixed embedding was set to 2 layers and the head and piston embedding is set to 1 layer. The grid scaling was usually used in compression stroke [29].



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Fig. 9. Grid control strategy in CONVERGE code

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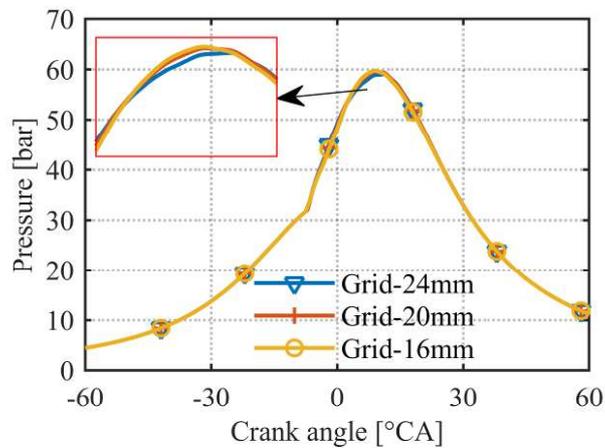
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The calculation time and calculation accuracy of CFD model were decided by mesh grid size [52]. To handle the relationship between time and accuracy, simulated in-cylinder pressures for 16, 20, and 24 mm base grids with grid control strategy were compared [62]. As it is shown in Fig. 10, the in-cylinder pressure trends of 16 and 20 mm are almost uniform and the in-cylinder pressure of 24 mm is lower than the 20 and 16 mm. Due to the large-bore and stroke of the engine, the small grid size causes the long calculation time. In this paper, the 20 mm base value grid was chosen to simulate the combustion process

310 with the adaptive mesh refinement and fixed embedding grid control strategy [28, 63].

311



312

313 Fig. 10. Comparison of in-cylinder pressure curve with different basic grids

314

315 The peak firing pressure and emissions products were tested and used to validate the accuracy of the  
 316 model. The 1-D simulation in-cylinder pressure curve was used to validate the 3-D simulation model. The  
 317 3-D engine simulation was performed by using the commercial CFD software package CONVERGE 2.4  
 318 [42]. The simulation started at IVC and ended at EVO, which means that only high pressure processes  
 319 were simulated. The port fuel injected natural gas was considered to be homogeneously mixed with air at  
 320 IVC [26]. The boundary, initial and operation conditions for the numerical simulation are illustrated in  
 321 Table 5.

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Table 5 Boundary, initial and operation conditions

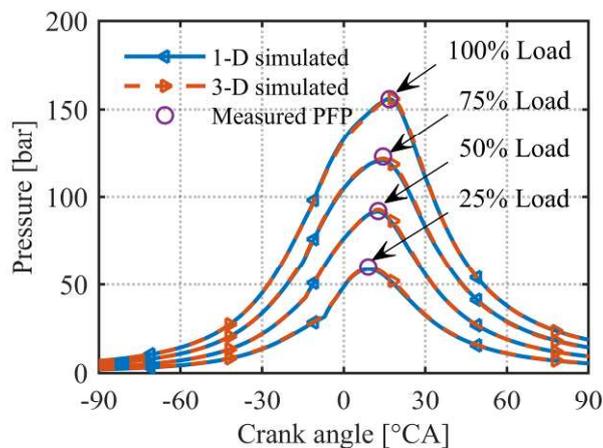
Terms	Unit	Value
Boundary conditions		
Head	K	553
Piston	K	523
Wall	K	433
Initial conditions		
Temperature at IVC	K	355
Pressure at IVC	bar	1.12

Turbulent kinetic energy	$\text{m}^2/\text{s}^2$	40
Turbulent dissipation	$\text{m}^2/\text{s}^3$	1720
Operation conditions		
Load	[-]	25%
SOI	$^{\circ}\text{BTDC}$	15
Speed	rpm	514

324

325 The engine speed was 514 r/min when operated at 25% load. The detailed parameters for modeling  
 326 and calibrating are reported in Table 5. The in-cylinder pressure and emissions products were tested and  
 327 used to validate the accuracy of the model. The comparison between the 3-D simulated and 1-D simulated  
 328 in-cylinder pressure profiles and measured peak firing pressure (PFP) are presented in Fig. 11. The trend  
 329 of the 3-D simulated results was in reasonable agreement with 1-D simulated results, but the 3-D  
 330 calculated peak firing pressure is slightly lower than the measured results. In addition, the comparison of  
 331 the key parameters between 3-D simulated and measured data are presented in Fig. 12. Where, the crank  
 332 angle of peak firing pressure (PFPCA) and total heat release (THR) were compared with the 1-D  
 333 simulated results and the PFP and  $\text{NO}_x$  were compared with the measured results. It can be inferred from  
 334 Fig. 8. that the maximum errors between simulated results and measured data are within 2%. It can be  
 335 concluded that the present model was capable of simulating the combustion process within the cylinder  
 336 accurately.

337

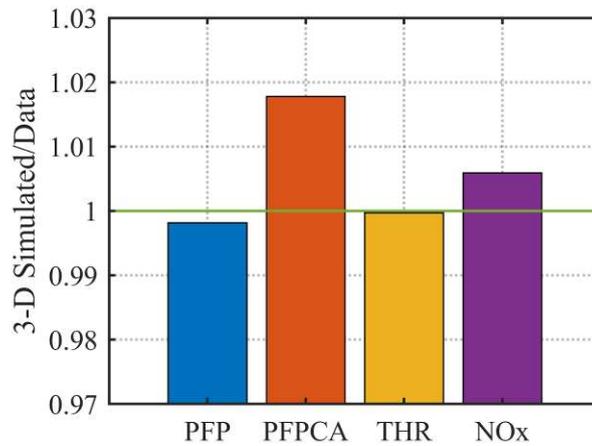


338

339 Fig. 11. Comparison between the 3-D simulated and 1-D simulated in-cylinder pressure profiles and

340  
341

measured peak firing pressure



342  
343

Fig. 12. Comparison of 3-D simulation and data values of key parameters

344

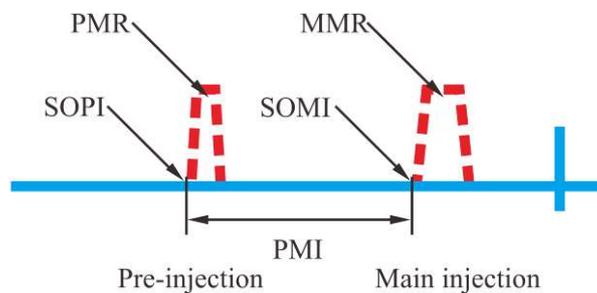
### 3. Pre-injection strategy and knock

345

#### 3.1. Pre-injection strategy

346

347 The parameters defined for the pre-injection research are as follows. The SOPI is the start of pre-  
348 injection, the PMR is the pre-injection mass ratio, the PMI is the pre-injection and main injection interval,  
349 the SOMI is the start of the main injection and the MMR is the main injection mass ratio. The schematic  
350 diagram of the pre-injection parameters is illustrated in Fig. 13. It can be inferred from Fig. 13 that the  
351  $PMI = SOPI - SOMI$  and the  $PMR = 1 - MMR$ .  
352  
353  
354



355

356

Fig. 13. Schematic diagram of pre-injection parameters

357

358 The parameters of the pre-injection strategy are shown in Table 6. It can be observed from Table 6  
 359 that Case 1 is the original single injection timing, Case 2 is the pre-injection timing strategy and Case 3 is  
 360 the pre-injection mass ratio strategy.

361

362

Table 6 Parameters of the pre-injection strategy

Case	Load [%]	SOPI [deg ATDC]	PMR [-]	SOMI [deg ATDC]	MMR [-]	Step [deg or -]
1	25	—	—	-15	1.0	—
2	25	-20 ~ -60	0.5	-15	0.5	10
3	25	-60	0.1 ~ 0.9	-15	0.9 ~ 0.1	0.2

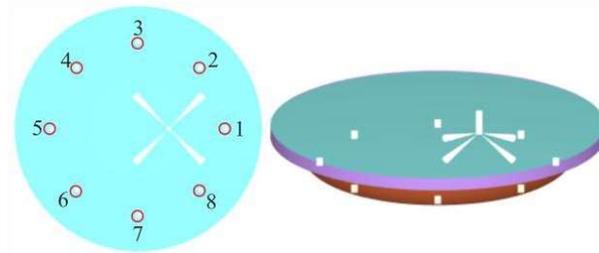
363

### 364 3.2. Pressure oscillation monitor and knock index

365

366 In order to monitor the pressure oscillations, the monitoring points (MP) were all placed near the  
 367 wall of the combustion chamber and away from the injector, as shown in Fig. 14.

368



369

Fig. 14. Schematic diagram of monitoring points

371

372 In order to quantify the phenomenon of knock, the knock index (KI) was introduced to define the  
 373 intensity of the knock [20, 46]. This parameter was defined as Eqs. (9).

$$374 \quad KI = \frac{1}{N} \sum_{i=1}^N PP_{\max, n} \quad (9)$$

375 Where the  $PP_{\max, n}$  is the difference between the peak pressure at monitoring points and the peak in-  
 376 cylinder pressure.

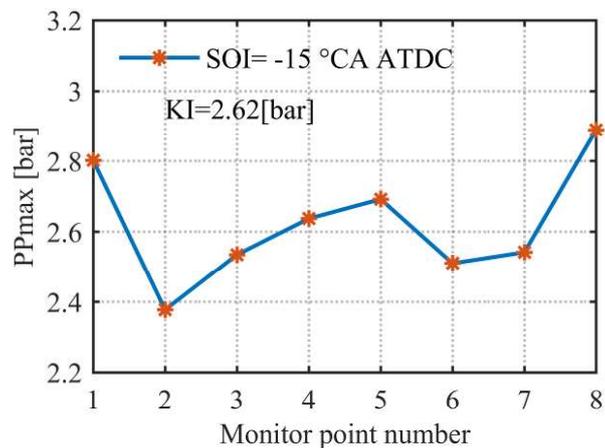
377

### 378 3.3. Analysis of cylinder pressure oscillation

379

380 In order to determine the limitation of KI, the knock of the original engine needs to be analyzed. The  
381 peak-to-peak values of each monitoring points are indicated in Fig. 15. It can be clearly seen from Fig.  
382 15. that the pressure at monitoring points No. 1 and No. 8 are the largest, and the pressure at the  
383 monitoring point No. 2 is the smallest. The main reason for the dramatic change in pressure at monitoring  
384 point 8 is that the pilot injector is not located in the center of the combustion chamber, which cause the  
385 flame to spread different distances. It can be calculated that the knock index KI is 2.62 bar. So the  
386 maximum KI in this paper is limited to 2.62 bar.

387



388

389 Fig. 15. Peak-to-peak pressure of the monitoring point and KI

390

## 391 4. Result and discussion

392

### 393 4.1. Knock analysis

394

395 Fig. 16 shows the KI in pre-injection. It can be seen in Fig. 16 (a) that the KI is lower than the base  
396 value when the SOPI = -30 and -50°C A, and the others SOPI are higher than the base value. The shorter  
397 injection interval causes KI to approach the base value at SOPI = -20 °C A. When the SOPI is after -  
398 30 °C A, the KI decreases as the SOPI is advanced. The KI increases when SOPI = -40 °C A and decreases

399 when the injection interval continues to increase due to the change of the combustion mode. As can be  
 400 seen from Fig. 16 (b), the KI changes very little when the pre-injection mass is relatively small, and is  
 401 greatest when the pre-injection mass ratio is 0.5. This is because the combustion is controlled by the main  
 402 injection fuel when the pre-injection mass ratio is small. The smaller pre-injection mass ratio equates to a  
 403 slightly earlier injection timing, so the KI change is small. When the pre-injection mass ratio is 0.5, it  
 404 results in unstable combustion because it is at the transition threshold of the combustion mode. When the  
 405 pre-injection mass ratio is less than 0.5, the combustion is the traditional diesel compression ignition  
 406 mode, when the pre-injection mass ratio is greater than 0.5, the combustion mode is the two-stage  
 407 autoignition mode. However, when PMR is 0.9, the KI increases significantly because the temperature  
 408 and pressure in the combustion chamber are lower during injection, and the injected fuel spreads around  
 409 due to the swirl in the combustion chamber. This causes the combustion to start only after the main  
 410 injection, resulting in a larger KI [15].

411

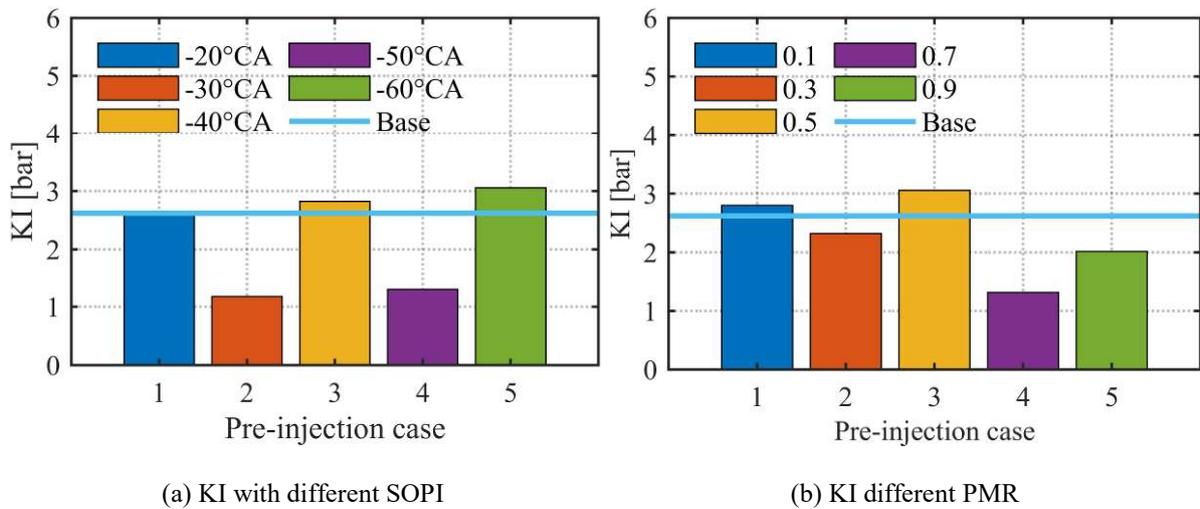
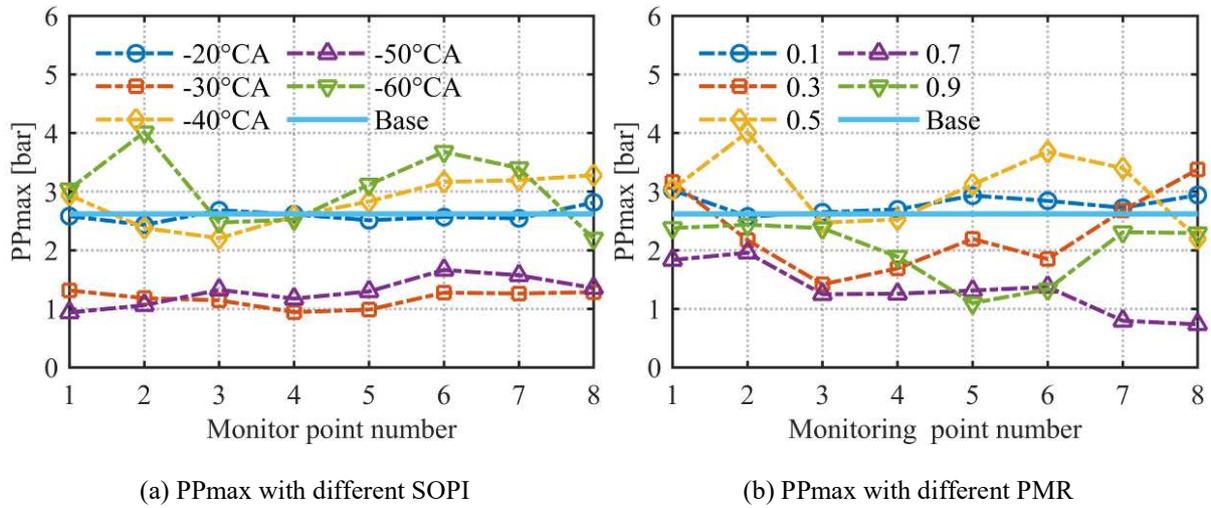


Fig. 16. Knock index

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413

414 The pressure peak-to-peak value of each monitoring points with pre-injection is shown in Fig. 17.  
 415 The points of polyline represent the maximum value of the pressure oscillation of each monitoring point.  
 416 It can be seen in Fig. 17 that the pressure peak-to-peak values of the monitoring points No. 2 was higher  
 417 than those of other monitoring points, indicating that the monitoring point of No. 6 is more prone to  
 418 knocking. The close pressure difference indicates steady combustion and uniform pressure transfer.



420

Fig. 17. Monitoring point pressure PPmax

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432

For further understanding of the in-cylinder combustion processes, the distribution of the  $\text{CH}_2\text{O}$  radical is shown in Fig. 18. The white line in Fig. 18 is the 1800K temperature contour, which represents the flame front. The  $\text{CH}_2\text{O}$  is one of the most important intermediates in the  $\text{CH}_4$  low temperature reaction, which is mainly distributed at the front of the flame, indicating that  $\text{CH}_2\text{O}$  is involved in the low temperature reaction [29]. The reaction rate of  $\text{CH}_2\text{O}$  directly influences the oxidation rate of methane, which affects the combustion process in the cylinder [61]. It can be seen from Fig. 18 (a) and (b) that when unstable combustion occurs, the distribution of  $\text{CH}_2\text{O}$  is far away from the 1800 K flame front. As can be seen from Fig. 18, the larger pre-injection interval to pre-injection mass ratio causes the fuel to adhere to the wall surface. This condition reduces KI, but causes the phenomenon of the wetted wall and limits the pre-injection strategy.

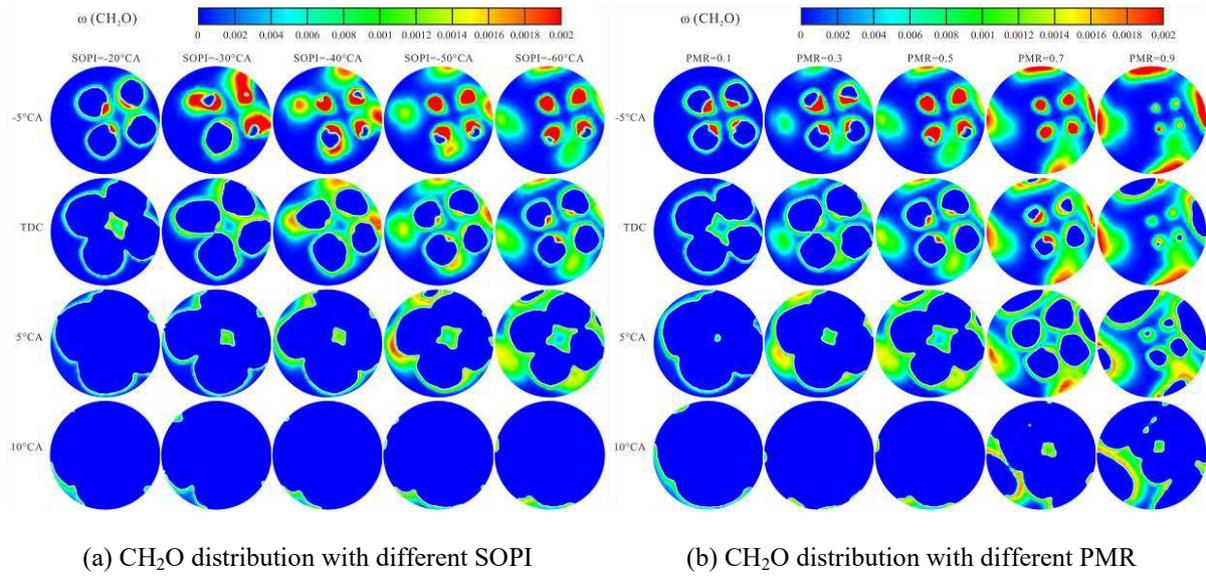


Fig. 18. In-cylinder CH<sub>2</sub>O distribution with different SOPI

433

434

#### 4.2. Combustion analysis

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445

The variation of the in-cylinder pressure curve is presented in Fig. 19. As can be seen from Fig. 19 (a), the peak firing pressure decreases and then increases as the injection interval increases. The timing of the peak firing pressure is delayed by the increase in the injection interval. As can be seen from Fig. 19 (b), the peak firing pressure is greatest when the pre-injection mass ratio is 0.5. As the pre-injection mass ratio continues to increase, the cylinder pressure profile remains the same. This is because when the pre-injection mass is larger, the pressure and temperature of the chamber are lower during injection, resulting in weaker combustion control by the main injection, and the combustion mode changes to the two-stage autoignition mode.

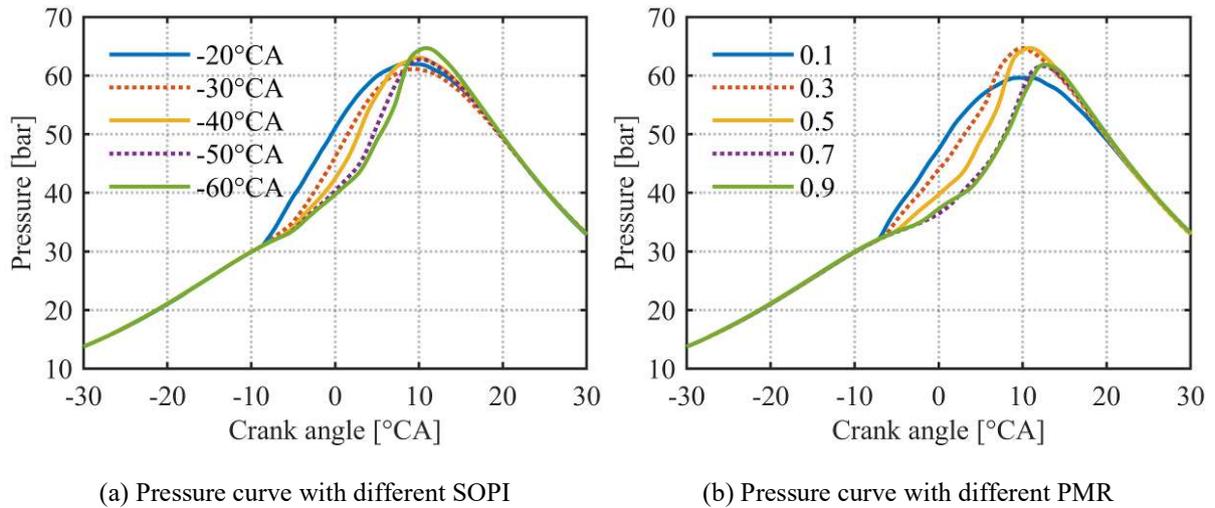


Fig. 19. In-cylinder pressure curve

446

447

448 Fig. 20 shows profiles of the heat release rate. It can be seen in Fig. 20 (a) that the advance of the  
 449 SOPI leads to the increased peak in heat release rate (HRR) and causes the HRR curve to change from a  
 450 single peak to twin peaks. Due to the complex combustion process of diesel-natural gas engines, the  
 451 different physicochemical properties of diesel and natural gas result in a significant combustion time  
 452 order of the two fuels [31]. When the injection interval is small (SOPI = -40~-30°CA), the advance pre-  
 453 injection timing causes the first peak lower and the second peak higher. When the injection interval is  
 454 large (SOPI = -60~-50°CA), the heat release rate shape becomes a single peak. As Fig. 20 (b) shows, the  
 455 critical parameter for combustion mode transition is that the pre-injection mass ratio is 0.5, and when less  
 456 than or greater than this ratio, the combustion beginning point is basically the same. The first peak is  
 457 dominated by pre-mixed fuel and the second by the burnable gas mixture. When the pre-injection interval  
 458 is large, the combustion chamber temperature and pressure during fuel injection are lower. This weakens  
 459 the spraying and evaporating process of the fuel, allowing for increased periods of ignition delay [52].  
 460 However, when the pre-injection timing is too early (SOPI = -60°CA) and the pre-injection mass ratio >  
 461 0.5, the phenomenon of wetted wall occurs under the action of the in-cylinder swirl due to the low  
 462 pressure in the combustion chamber and the long mixing time [26]. This causes the pre-injected fuel to  
 463 burn near the wall surface and leads the unstable combustion [64, 65].

464

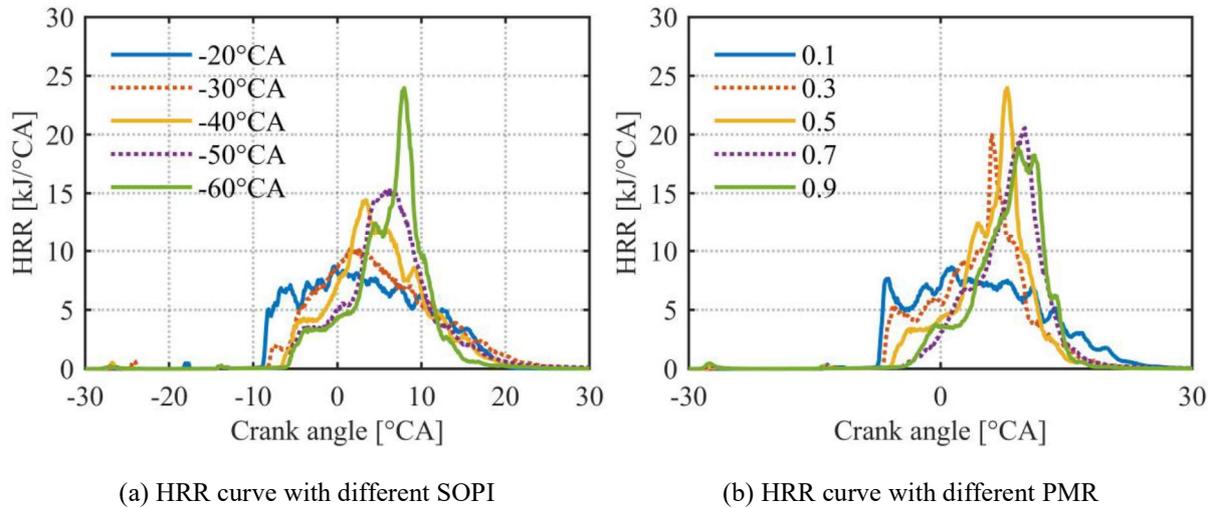


Fig. 20. Heat release rate curve

465

466

467 Fig. 21 shows the variation of IMEP. It can be seen from Fig. 21 (a) that IMEP increases with the

468 advance of SOPI. However, when SOPI is  $-60^{\circ}\text{CA}$ , IMEP decreases. Fig. 21 (b) shows the IMEP with

469 different PMR. It can be seen from Fig. 21 (b) that the IMEP is lowest at a pre-injection mass ratio of 0.1.

470 The smaller pre-injection mass ratio is equivalent to slightly advancing the injection timing of a single

471 injection, and the combustion is still controlled by the main injection, so the IMEP is smaller. IMEP is

472 greatest when the pre-injection mass ratio is 0.3. This is because the large injection intervals allow for

473 enough time for the fuel to mix. As the pre-injection mass ratio continues to increase, the main injection

474 fuel control capacity decreases, causing the combustion phase to be delayed, which leads to a lower IMEP.

475 This is because during fuel injection, the lower temperature and pressure of the combustion chamber with

476 the longer mixing time results in the phenomenon of the wetted wall [51].

477

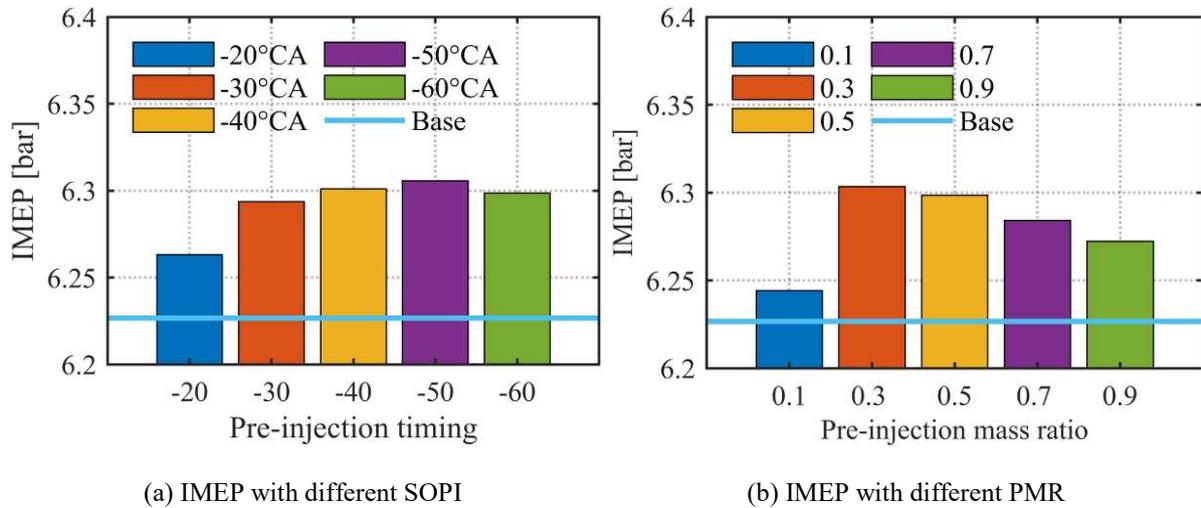


Fig. 21. Indicated mean effective pressure

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### 4.3. Emissions analysis

481

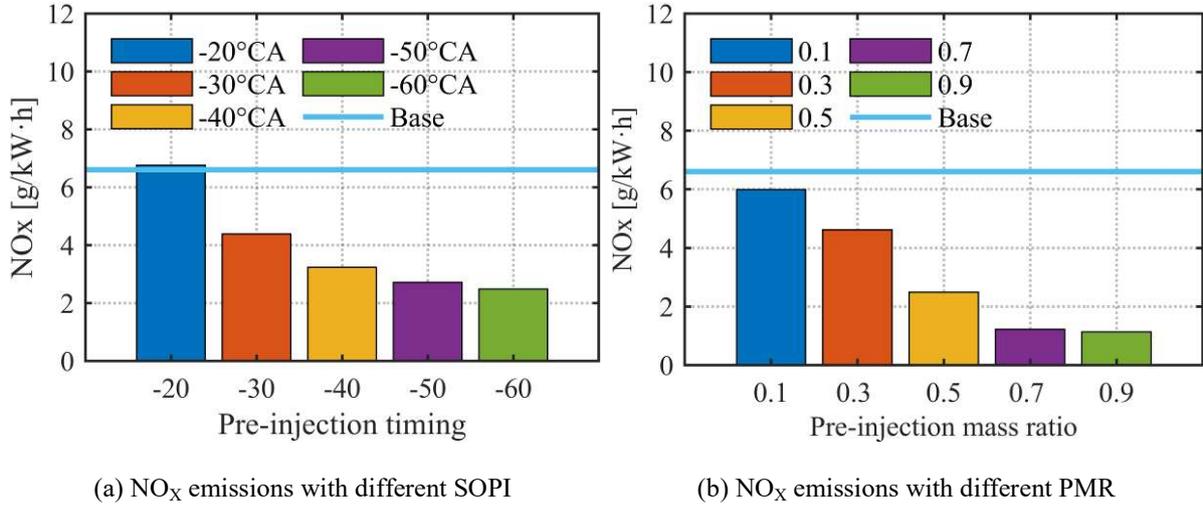
482 The soot generation is higher in conventional diesels and smaller in dual-fuel engines, especially at  
 483 higher rate of natural gas substitution [13, 15]. In this paper, the analysis focuses on  $\text{NO}_x$ , THC and CO  
 484 emissions because of the high rate of natural gas substitution ( $> 95\%$ ).

485 Fig. 22 shows the comparison of indicated  $\text{NO}_x$  emissions. it can be seen from the Fig. 22 that at  
 486 smaller pre-injection intervals (SOPI =  $-20^\circ\text{CA}$ ), the advance of the injection timing leads to an increase  
 487 in  $\text{NO}_x$  due to the larger injection ratio (PMR = 0.5), which is equivalent to the advance of the single  
 488 injection timing. When a smaller pre-injection interval (SOPI =  $-20^\circ\text{CA}$ ) is ignored,  $\text{NO}_x$  emissions are  
 489 reduced by both increasing the pre-injection mass ratio and increasing the pre-injection interval. This is  
 490 because the pre-injection strategy increases fuel mixing time, resulting in a wider distribution of fuel drip  
 491 and lowering the maximum combustion temperature in the cylinder.

492 Fig. 23 shows the temperature distribution in the combustion chamber. The temperature profile  
 493 provides a visual representation of the location of the high-temperature region in the combustion chamber  
 494 and it is important for the analysis of  $\text{NO}_x$  emissions. The longer mixing time between the pre-injected  
 495 diesel and natural gas mixture reduces the area of uneven local fuel concentration in the cylinder, which  
 496 inhibits  $\text{NO}_x$  generation and thus reduces  $\text{NO}_x$  emissions. It can be seen from Fig. 23 that the high-

497 temperature region decreases with increasing the pre-injection ratio and pre-injection interval when using  
 498 the pre-injection strategy [53].

499



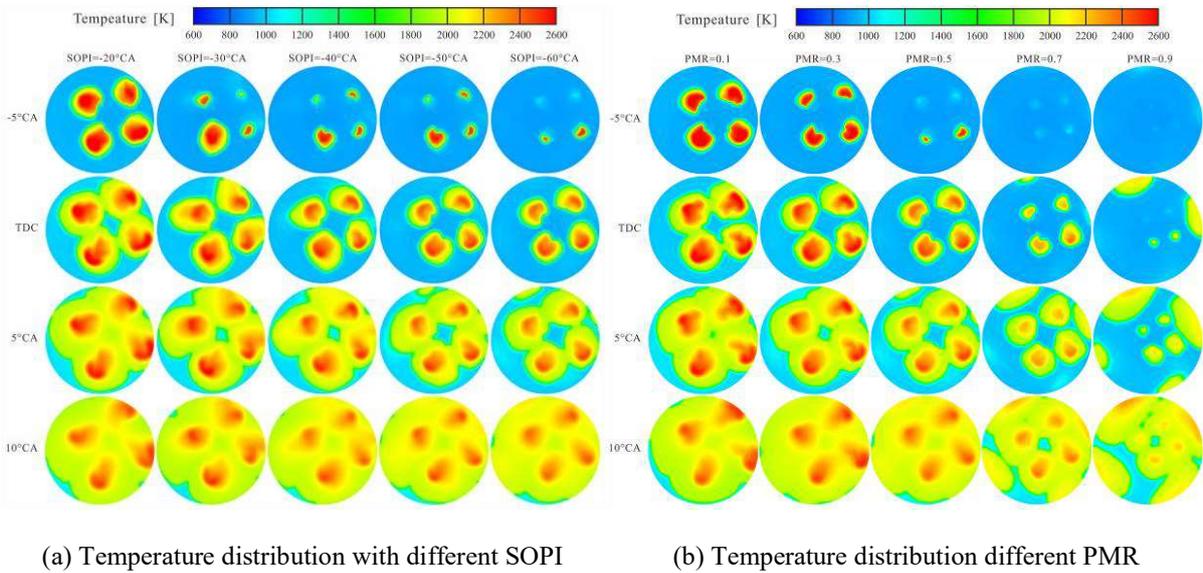
(a) NO<sub>x</sub> emissions with different SOPI

(b) NO<sub>x</sub> emissions with different PMR

500

Fig. 22. Indicated NO<sub>x</sub> emissions

501



(a) Temperature distribution with different SOPI

(b) Temperature distribution different PMR

502

Fig. 23. In-cylinder temperature distribution

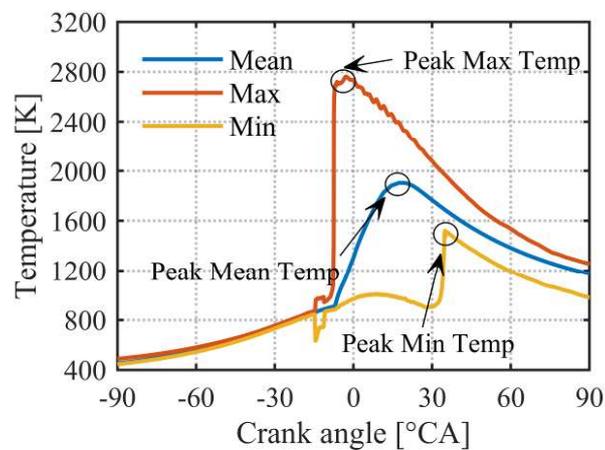
503

504 The schematic diagram of temperature curve is presented in Fig. 24. As shown in Fig. 24, the  
 505 temperature curve includes three curves which are mean temperature, maximum temperature and  
 506 minimum temperature of the chamber. If the combustion chamber is divided into burned zone and  
 507 unburned zone, the maximum temperature in Fig. 24 represents the temperature of the burned zone and

508 the minimum temperature in Fig. 24 represents the temperature of unburned zone and the mean  
 509 temperature represents the mean value of the in-cylinder temperature. According to previous studies,  $\text{NO}_x$   
 510 generation is mainly in the burned zone, so the burned zone temperature is particularly important for  
 511 measuring  $\text{NO}_x$  generation [66]. The peak maximum temperature, peak mean temperature and peak  
 512 minimum temperature are compared from Fig. 25. It can be seen from Fig. 25 that the peak maximum  
 513 temperature decreases with increasing pre-injection interval and pre-injection mass ratio. The pre-  
 514 injection interval has a significant effect on the peak maximum temperature, while the pre-injection mass  
 515 ratio has a minor effect on the peak maximum temperature.

516 Fig. 26 shows the  $\text{NO}_x$  distribution in the combustion chamber. The local high combustion  
 517 temperature regions are relatively wide which results in relatively higher  $\text{NO}_x$  emissions. As can be seen  
 518 from Fig. 26, the  $\text{NO}_x$  distribution region in the combustion chamber is consistent with temperature,  
 519 indicating that temperature is an important factor in the influence of  $\text{NO}_x$ .  $\text{NO}_x$  production is particularly  
 520 small when the pre-injection mass ratio is large and pre-injection is positive [13].

521

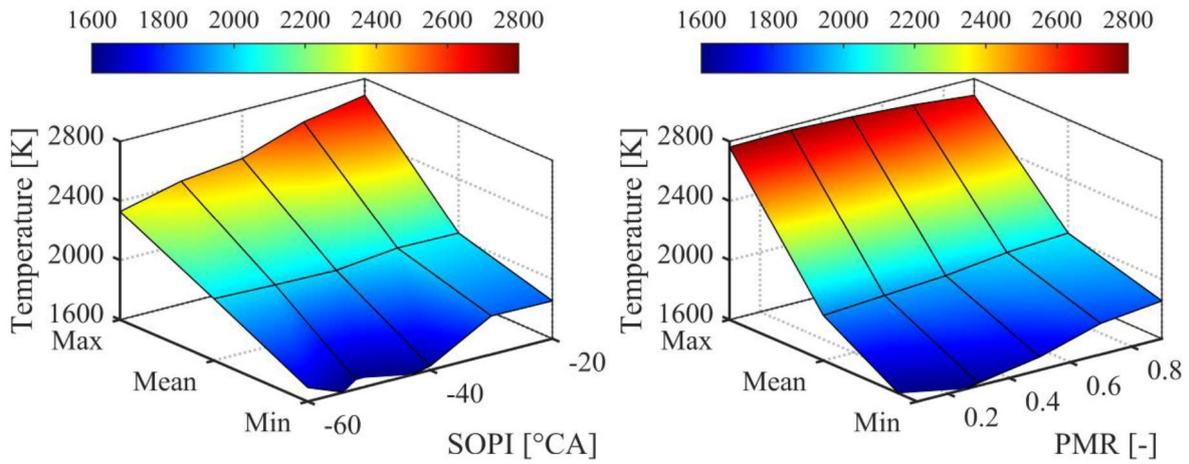


522

523

Fig. 24. Schematic diagram of temperature curve

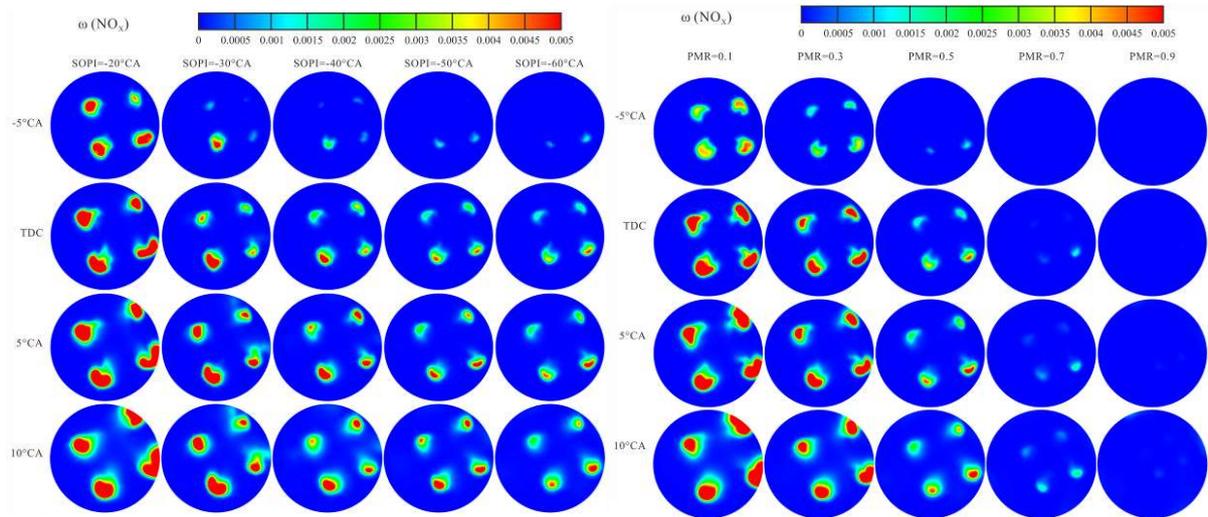
524



(a) Temperature comparison with different SOPI      (b) Temperature comparison with different PMR

525      Fig. 25. Comparison of maximum temperature, average temperature and minimum temperature

526



(a) NO<sub>x</sub> distribution with different SOPI      (b) NO<sub>x</sub> distribution with different PMR

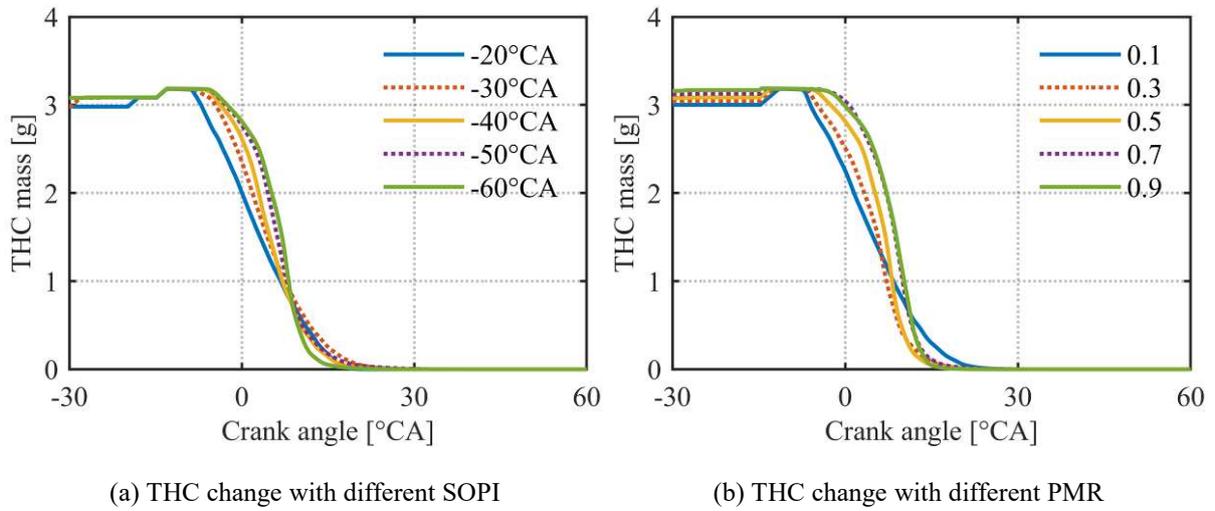
527      Fig. 26. In-cylinder NO<sub>x</sub> distribution

528

529      The hydrocarbons is one of the main emissions of dual-fuel engines in ships, and in dual-fuel  
 530 engines the main component of hydrocarbons is methane. Fig. 27 shows the mass change of total  
 531 hydrocarbons (THC). As can be seen from Fig. 27, THC consumption is very slow before the TDC and  
 532 rises sharply around 10 °CA with the pre-injection interval and pre-injection mass ratio increase. This is  
 533 because at larger pre-injection intervals and pre-injection mass ratio, the injected fuel cannot burn  
 534 immediately due to the lower temperature and pressure in the combustion chamber. Advancing pre-

535 injection timing leads to leaner diesel and natural gas-air mixture formation which causes the combustion  
 536 to start after the main fuel injection. When the pre-injection mass ratio is larger, the pre-injection fuel is  
 537 distributed in the natural gas mixture. This promotes the production of flammable products in the middle  
 538 of the flammable mixture, increasing the ignition area of the gas. The accelerated rate of combustion of  
 539 the gas mixture has resulted in a higher utilization of natural gas. The combustion mode also transforms  
 540 from the traditional diesel compression ignition mode to the two-stage autoignition mode [13].

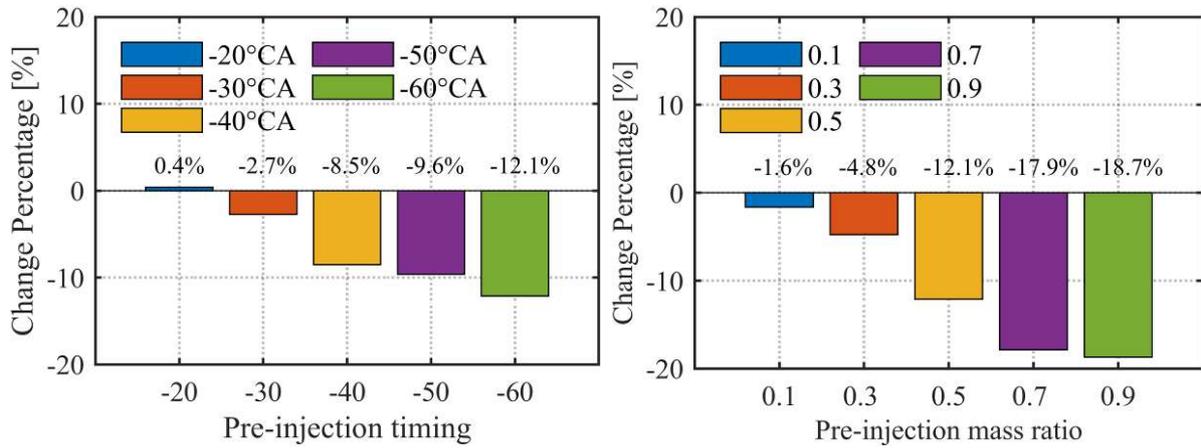
541



542 Fig. 27. Total hydrocarbon mass change

543

544 The changes of the CO are illustrated in the Fig. 28. It can be seen from Fig. 28. that compared to  
 545 single injection mode, pre-injection considerably reduces the CO emissions. Further advancing pre-  
 546 injection timing weakens the effect of pre-injected fuel on ignition and larger pre-injection mass and early  
 547 pre-injection timing caused the longer mixture time for diesel and air which decreases the CO emissions.



(a) CO change percentage with different SOPI

(b) CO change percentage with different PMR

Fig. 28. CO change percentage comparison

548

549

## 550 5. Conclusions

551

552 In the present study, a large marine four-stroke DF engine was thoroughly investigated by using the  
 553 CONVERGE software to reveal its knock, combustion and emissions characteristics. The effects of pre-  
 554 injection timing and pre-injection mass ratio on knock, combustion and emissions of the investigated  
 555 engine has been studied numerically. The major concluding remarks from this study are summarized as  
 556 follows.

557 1) The different combustion modes can be achieved by advancing the pre-injection time and  
 558 increasing the pre-injection mass ratio. The critical parameters for the combustion mode transition were  
 559  $SOPI = -40^\circ CA$  and  $PMR = 0.5$ , respectively. When the  $PMI > 25^\circ CA$  and  $PMR > 0.5$ , the heat release  
 560 rate shape becomes a single peak and the combustion phase shift backward.

561 2) When the KI is smaller, the difference between each measurement point is also smaller. KI  
 562 decreases as the injection interval and pre-injection mass ratio increase when in the traditional diesel  
 563 compression ignition mode, but reverses when in two-stage auto-ignition mode. When  $PMR = 0.5$  and  
 564  $SPOI = -60^\circ CA$ , the pressure difference at each measurement point is the largest and the KI is also the  
 565 largest. The smallest KI can be obtained when the  $SOPI = -30^\circ CA$  and  $PMR=0.5$ , respectively.

566 3) The  $NO_x$  emissions decrease with increasing injection intervals and pre-injection mass ratio due  
 567 to the longer fuel mixing time and lower maximum combustion temperature. The trend in CO emissions

568 is consistent with  $\text{NO}_x$  for different injection strategies. At  $\text{PMR}=0.5$ , the reduction in CO emissions  
569 becomes greater due to change of the combustion mode. The THC consumption accelerates with  
570 increasing injection intervals and pre-injection mass ratio, indicating that a proper pre-injection can  
571 reduce hydrocarbon emissions. However, when  $\text{SOPI} = -60^\circ\text{CA}$ ,  $\text{PMR} = 0.7\sim 0.9$ , the consumption rate is  
572 almost the same.

573 4) In all pre-injection strategies, IMEP is higher than a single injection. The IMEP increases with  
574 increasing pre-injection interval and decreases with increasing pre-injection mass ratio when large pre-  
575 injection intervals and small pre-injection mass ratio are not considered. The maximum can be achieved  
576 when the  $\text{PMR} = 0.5$  and the  $\text{SOPI} = -50^\circ\text{CA}$  or the  $\text{PMR} = 0.3$  and the  $\text{SOPI} = -60^\circ\text{CA}$ .

577 5) Among the calculated cases, when  $\text{NO}_x$ , KI and IMEP are considered together, the best pre-  
578 injection parameters are  $\text{SOPI} = -50^\circ\text{CA}$  and  $\text{PMR} = 0.5$ . When considering KI alone, the lowest KI can  
579 be obtained when  $\text{SOPI} = -60^\circ\text{CA}$  and  $\text{PMR} = 0.7$ . It can be reasonably estimated the best parameters are  
580  $\text{SOPI} = -50^\circ\text{CA}$  and  $\text{PMR} = 0.3$  when the goal is to reduce  $\text{NO}_x$  emissions without sacrificing economy  
581 and dynamics, and consider the limitation of KI and phenomenon of the wetted wall.

582 In conclusion, the present study provides the basis for the pre-injection strategy of DF engines and  
583 the results contributed to the better understanding the improvement of knocking, combustion and  
584 emissions by pre-injection strategy. The law of influence of the pre-injection strategy on the phenomenon  
585 of knock is explained, and a method for determining the phenomenon of knock is determined, which is  
586 also applicable to the determination of the phenomenon of knock of DF engines at high load. The current  
587 investigation helps to get a better understanding of the theoretical basis for the pre-injection strategy,  
588 improving the actual engine combustion stability, and avoiding the phenomenon of knock of the DF  
589 engines. In future work, machine learning algorithms will be used to model pre-injection strategies, and  
590 genetic algorithms will be combined with machine learning models to optimize pre-injection parameters.

591

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593

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596

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598

599

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