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Additional Information

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31  
32 **Abstract**

33 Focusing on the dual-mode dual-fuel (DMDF) combustion concept, a combined optimization of the piston bowl  
34 geometry with the fuel injection strategy was conducted at various loads. An improved genetic algorithm was  
35 introduced in this study, which is superior in searching for the global optimal solutions. The optimal piston bowl  
36 shape coupled with the corresponding injection strategy was summarized at the various loads. The results show that  
37 the piston bowl geometry optimization can further improve the thermal efficiency with 1.4%, 4.4%, and 1.4%  
38 percentage points for the low, mid, and high loads, respectively. An indicated thermal efficiency up to 51.8% can be  
39 realized at mid load. Meanwhile, for all the optimal cases, NO<sub>x</sub> and soot emissions can meet the Euro VI limits.

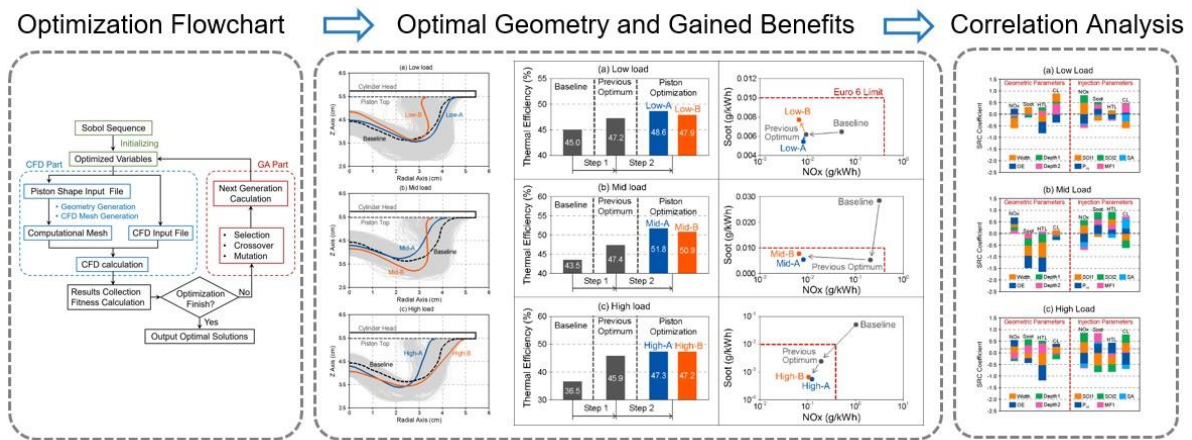
40 At low and mid loads, both the open and re-entrant type piston bowl can be equipped, while the high load only  
41 prefers the open type piston bowl for the DMDF mode. The re-entrant type or deep piston bowls are superior in  
42 organizing strong in-cylinder flow, which is beneficial for the fuel/air mixing. The open type or shallow piston bowls  
43 are helpful for reducing the heat transfer losses owing to the less heat transfer surface area. Furthermore, a correlation  
44 analysis was conducted to investigate the sensitivity of engine performance to the piston geometric parameters and

45 injection parameters. It is concluded that the fuel injection event becomes more important for managing the engine  
 46 performance as load increases. Among the injection parameters, the influence of the fuel injection timings and  
 47 injection pressure on engine performance is more obvious. The piston geometric parameters play more significant  
 48 roles in the heat transfer losses than the injection parameters for all loads. Among the geometric parameters, the most  
 49 influential parameters are the width and open extent of the piston bowl. The heat transfer loss energy fraction can be  
 50 well decreased with a wider and more open piston bowl.

51 **Keywords:** Piston bowl geometry optimization; Dual-mode dual-fuel (DMDF); Genetic algorithm; Fuel efficiency;  
 52 Correlation analysis

53

54 **Graphical abstract**



55

56

## Nomenclature

1D	one-dimensional	IVC	intake valve closing
3D	three-dimension	LHV	lower heating value
ATDC	after top dead center	LTC	low-temperature combustion
CA50	50% burn point	MF1	mass fraction of the first injection
CDC	conventional diesel combustion	NSGA	non-dominated sorting genetic algorithm
CFD	computational fluid dynamics	NO <sub>x</sub>	nitrogen oxides
CL	combustion losses	OE	Open Extent
CO	carbon monoxide	$p_{inj}$	injection pressure
DI	direct injection	$p_{ivc}$	inital pressure at IVC timing
D MDF	dual-mode dual-fuel	$p_{max}$	maximum in-cylinder pressure
DOE	design of experiment	PPC	partially premixed combustion
DPF	diesel particulate filter	PPRR	peak pressure rise rate
EGR	exhaust gas recirculation	PR	premix ratio
EISFC	equivalent indicated specific fuel consumption	RCCI	reactivity controlled compression ignition
EPA	Environmental Protection Agency	RI	ringing intensity
GA	genetic algorithm	SA	spray angle
GCR	geometric compression ratio	SCR	selective catalytic reduction
HRR	heat release rate	SOI	start of injection
HC	hydrocarbon	SOI1	start of injection timing for first pulse
HCCI	homogeneous charge compression ignition	SOI2	start of injection timing for second pulse
HTL	heat transfer losses	SRC	Spearman Rank Correlation
HTR	heat transfer rate	TDC	top dead center
ICE	internal combustion engine	$T_{ivc}$	initial temperature at IVC timing
IMEP	indicated mean effective pressure	VVT	variable valve timing
ISFC	indicated specific fuel consumption		

57

58

## 59 1. Introduction

60 The increasingly stringent emission regulations and urgent energy shortage are bringing huge challenges for the  
61 internal combustion engine (ICE) research community. Improving fuel economy and eliminating engine-out  
62 emissions are still the major objectives and main investigation fields for ICE researchers. Currently, the selective  
63 catalyst reduction (SCR) and diesel particulate filter (DPF) systems have been widely adopted by engine  
64 manufacturers as the aftertreatment devices for decreasing nitrogen oxides ( $\text{NO}_x$ ) and soot emissions, respectively.  
65 Although their effectiveness has been demonstrated, the engine layout complexity and cost are increased as well [1].  
66 Alternatively, the low-temperature combustion (LTC) strategy [2] was proposed, which yields great potential of  
67 reducing  $\text{NO}_x$  and soot emissions while maintaining pleasant fuel economy owing to the characteristics of  
68 homogeneous-mixing and low-temperature combustion process.

69 Among the LTC modes, reactivity controlled compression ignition (RCCI) [3] concept attracts more scientific  
70 interest due to the flexible control over the combustion process with the dual-fuel system. In RCCI mode, the fuel  
71 concentration and reactivity stratification can be accomplished relying on delivering the low-reactivity fuel by port  
72 fuel injection (PFI) and the high-reactivity fuel by in-cylinder direct injection (DI), respectively. By adjusting the  
73 low-reactivity fuel percentage and the direct injection event, the fuel distribution and reactivity can be tuned, and a  
74 flexible operation in a wide operating range can be realized [4]. In spite of this, the RCCI strategy is still facing the  
75 problems of low combustion efficiency at low load [5, 6] and serious engine noise at high load [7]. Thus, the  
76 improvement of the RCCI strategy over a wide operating range is still needed.

77 Up to now, many investigations focus on the extension of the RCCI operation range. Lim et al. [8] found that  
78 extremely low  $\text{NO}_x$  and soot emissions, as well as the indicated thermal efficiency of 48.7% can be reached for a  
79 gasoline/diesel RCCI engine at high load up to 21 bar of the indicated mean effective pressure (IMEP). Wang et al.  
80 [9] demonstrated the effectiveness of exhaust gas recirculation (EGR) rate for preventing excessively high peak

81 pressure rise rate (PPRR) and extending the RCCI mode to higher loads. Meanwhile, it was found that the  
 82 employment of gasoline/diesel dual-fuel RCCI mode at mid and high loads can maintain ultra-low NO<sub>x</sub> and soot  
 83 emissions, while the diesel LTC strategy with single fuel injection is more attractive for low load conditions.

84 Molina et al. [10] extended the RCCI operating range by employing a multiple direct-injection strategy  
 85 combined with the Miller cycle. At low load, the double injection strategy was used for managing the combustion  
 86 phasing and emissions. At high load, the injection shifts into a single injection for triggering the ignition and  
 87 maintaining mild combustion. Xu et al. [11, 12] optimized the key parameters of an RCCI engine couple with the the  
 88 variable valve timing (VVT) and variable compression ratio (VCR) strategies at various load conditions. The results  
 89 indicated that the Euro VI limit can be well maintained over the whole load range, whereas the trade-off of the NO<sub>x</sub>  
 90 and soot emissions at high load is difficult to solve. Mikulski et al. [13] found that early intake valve closing is  
 91 beneficial for the RCCI operation at high load, whereas retarding the intake valve opening timing can reduce  
 92 combustion losses.

93 Benajes et al. [14] indicated that 80% of the nominal operating range for conventional diesel engines can be  
 94 covered by the RCCI operation by employing appropriate fuel ratio, EGR rate, and intake temperature, while the  
 95 PPRR limit will not be surpassed. Based on that study, a dual-mode dual-fuel (DMDF) concept was proposed by  
 96 Benajes et al. [15]. In the DMDF concept, the combustion mode was shifted regarding the engine load. At low load,  
 97 the highly-premixed RCCI operation was employed for enhancing the engine efficiency and obtaining low levels of  
 98 emissions. At high load, the combustion mode was switched to diffusive combustion for slowing down the  
 99 combustion rate and meeting the engine mechanical restriction. Recently, a series of efforts were made for the  
 100 development of the DMDF concept, as summarized in Table 1.

101  
 102 Table. 1. A Summary of the main papers published on DMDF combustion mode

Reference	Contents of the research	Main Conclusions
Benajes et al.	The DMDF concept was proposed featuring	<ul style="list-style-type: none"> <li>The DMDF concept can fulfill the EURO</li> </ul>

[15] (2017)	<p>that the combustion strategy changes as engine load increases.</p> <ul style="list-style-type: none"> <li>• At low loads with the indicated mean effective pressure (IMEP) lower than 8 bar, a fully premixed RCCI strategy is employed;</li> <li>• When engine load rises up to 15 bar, the combustion strategy is switched to highly premixed RCCI mode;</li> <li>• At full load operation, the diffusive dual-fuel combustion is employed.</li> </ul>	<p>VI NO<sub>x</sub> limit up to 14 bar IMEP;</p> <ul style="list-style-type: none"> <li>• Above 5 bar IMEP, the smoke emissions exceed the EURO VI standards for diesel engines, but the majority of the engine map can fulfill the smoke levels below 1 FSN.</li> </ul>
Benajes et al. [16] (2018)	<p>Comparison of the performance and emissions of two dual-mode combustion concepts over different driving cycles using different fuel combinations.</p>	<p>The dual-mode concept has a potential to be implemented in flexible-fuel engines.</p>
García et al. [17] (2019)	<p>Investigation of the effects of the octane number of the low-reactivity fuel at representative operating conditions over the DMDF engine map.</p>	<p>The characteristics of the low-reactivity fuel in the DMDF concept have a major impact on the combustion evolution in a wide range of engine load, speed, low-reactivity fuel fraction, dilution level, and combustion regime.</p>
Macián et al. [18] (2019)	<p>Investigation of the effect of the low-pressure exhaust gas recirculation (LP-EGR) on the gaseous and particle emissions of the DMDF concept fueled with standard gasoline and diesel.</p>	<ul style="list-style-type: none"> <li>• In the fully premixed RCCI mode, the application of the LP-EGR results in high hydrocarbon (HC) and carbon monoxide (CO) emissions;</li> <li>• For the other combustion modes in the DMDF concept, a reduction of the analyzed pollutants is demonstrated with the employment of the LP-EGR compared with the CDC mode.</li> </ul>
Xu et al. [19] (2020)	<p>Optimization of the operating parameters related to the intake condition and fuel injection strategy for strengthening the engine performance of the DMDF concept fueled with gasoline and diesel fuel at various load conditions.</p>	<p>Gross indicated thermal efficiency above 45% is achieved, and the NO<sub>x</sub> and soot emission can be maintained under the Euro VI standard for the whole load range.</p>
García et al. [20] (2020)	<p>Exploring the feasibility of using the fuel blend of oxymethylene ether (OME<sub>x</sub>) and diesel as the high-reactivity fuel instead of pure diesel in the DMDF concept for reducing the</p>	<p>The OME<sub>x</sub>-diesel blends with an OME<sub>x</sub> mass content greater than 70% are able to meet the Euro VI NO<sub>x</sub> standard with ultra-low soot levels (&lt; 0.01 g/kWh) up to 80% engine load.</p>



	lifecycle CO <sub>2</sub> emission.	
García et al. [21] (2020)	Exploration of suitable injector configuration and fuel injection strategy for the DMDF concept with diesel and OME <sub>x</sub> respectively as the high-reactivity fuels.	<ul style="list-style-type: none"> <li>• The long injection durations of OME<sub>x</sub> resulted from its low lower heating value is handled with the employment of the injectors with higher flow rate capacity.</li> <li>• The trade-off relationship between engine-out emissions and the mixing capacity of the injection system is solved, while the engine performance is not significantly affected.</li> </ul>

103

104 Up to date, the DMDF strategy demonstrates superior advantages for balancing load extension and performance  
105 improvement. It has been recognized as a promising dual-fuel combustion concept to satisfy future fuel consumption  
106 and emission regulations [17]. However, for the current DMDF strategy, there still exist some aspects to be further  
107 improved, among which the piston bowl geometry optimization is the most urgent. At present, the piston bowl  
108 geometry for the DMDF strategy is empirically determined. It is well known that the piston bowl geometry can exert  
109 significant influences on engine performance. Moreover, the interactions between the piston bowl structure and the  
110 injection event are crucial for the fuel/air mixture formation and combustion event for the dual-fuel combustion mode.  
111 Thus, the combined optimization of the piston bowl shape with the fuel injection parameters is needed to further  
112 enhance the DMDF combustion characteristics.

113 Up to now, many investigations have been conducted for studying the effects of the piston bowl geometry and  
114 searching for the optimal bowl shape for the engines with advanced combustion concepts. Dempsey et al. [22]  
115 compared the traditional re-entrant type with a modified shallow type piston based on an RCCI engine fueled with  
116 different fuel combinations. It was concluded that the shallow type piston yields better engine efficiency due to lower  
117 heat transfer losses. Similar results were also reported by Park et al. [23] that the shallow type piston bowl can  
118 contribute to a 35% improvement of the gross indicated thermal efficiency. Xu et al. [24] performed an investigation  
119 to study the joint effects of the bowl shape and injection timing based on the partially premixed combustion (PPC)

120 mode and homogeneous charge compression ignition (HCCI) mode. The results indicated that the piston with a  
121 stepped-lip shape is favorable for solving the low-load cold start problem in terms of decreasing the intake  
122 temperature requirement, which is owing to the fact that the fuel-rich regions can be produced in the stepped-lip  
123 piston bowl. Moreover, it was found that the effect of spray/wall interaction is important when the combustion mode  
124 shifts from HCCI to PPC. Nazemian et al. [25] optimized the piston bowl geometry of an RCCI engine by utilizing  
125 CONVERGE software combined with the design of experiment (DOE) method based on the second law of  
126 thermodynamics, and the effects of the main piston bowl shape parameters, including the piston bowl sizes, pip height,  
127 and top land height on exergy destruction were discussed. It was reported that the influence of the bowl diameter and  
128 bowl depth were the most significant of the exhaust heat recovery. The optimization study performed by Lee et al.  
129 [26] indicated that a 9% improvement of fuel consumption with simultaneously reduced NO<sub>x</sub> and soot emissions can  
130 be attained with a shallow type piston bowl and a narrow injection angle for a gasoline/diesel dual-fuel engine.

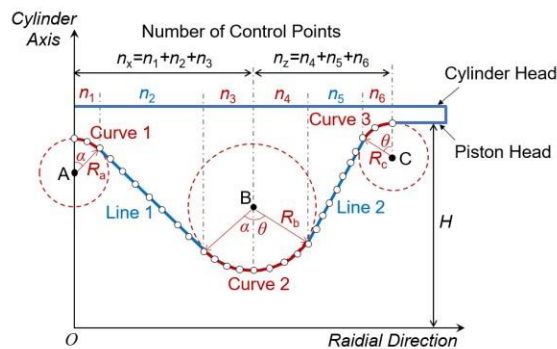
131 From the above literature review, it is confirmed that further optimization of the piston bowl shape used for the  
132 DMDF strategy can lead to potential improvements in fuel efficiency and engine-out emissions. Moreover, up to date,  
133 there have been few studies reporting the piston bowl geometry optimization over a wide load range for the engines  
134 with advanced combustion modes. Thus, in this study, the combined optimization of the piston bowl shape parameters  
135 with the fuel injection strategy was conducted over a wide load range for the DMDF mode based on an improved  
136 genetic algorithm integrated with the computational fluid dynamics (CFD) simulation. Then, the optimal piston bowl  
137 shape coupled with the injection strategy was summarized at different loads. Furthermore, a correlation analysis was  
138 conducted to investigate the sensitivity of engine performance to the geometric parameters and injection parameters,  
139 which can guide the engine structure design.

140

141 2. Computational Method

142 2.1. Generation of the Piston bowl geometry and computational mesh

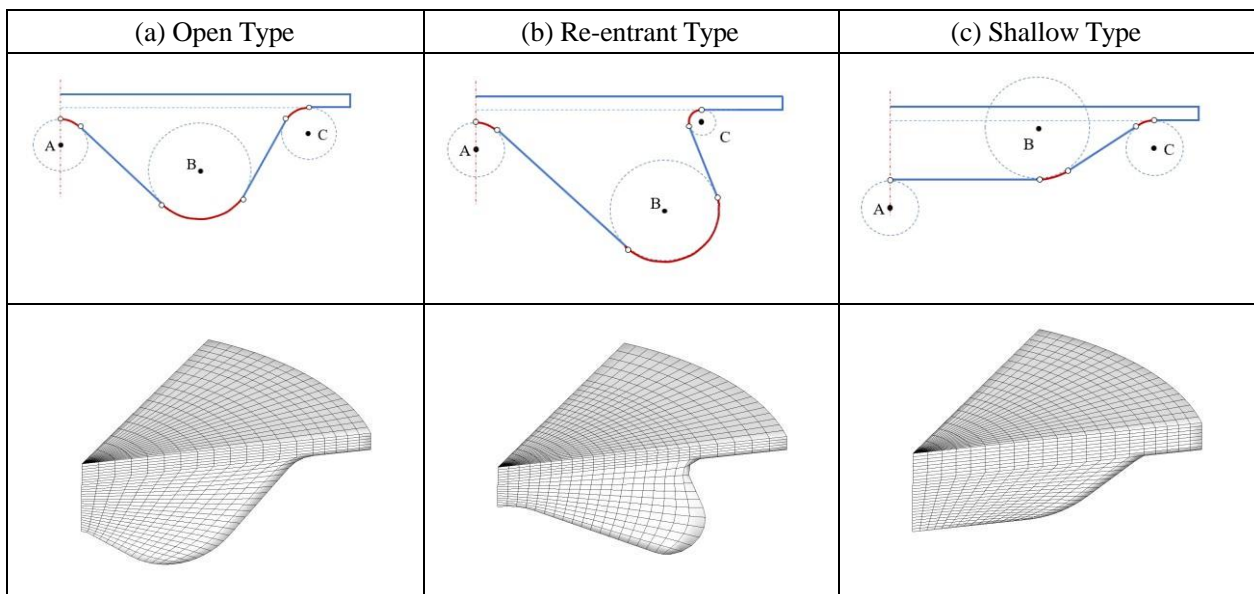
143 In this study, the shape of the piston bowl is generally described using two straight lines (*i.e.*, Line 1 and Line 2) and three circle curves (*i.e.*, Curve 1, Curve 2, and Curve 3) according to the work of Badra et al. [27]. The straight lines and circle curves are represented by the blue and red lines respectively in Fig. 1. It is comprehensible that the shape is determined by the location of circles A, B, and C, as well as their common tangent lines. Thus, the controllable parameters contain the  $X$  and  $Z$  locations of the circle center points A, B, and C, as well as the radius of the three circles, *i.e.*,  $R_a$ ,  $R_b$ , and  $R_c$ . Compared with the traditional method, in which the piston bowl shape is described by the Bezier Curve, the control variables are simplified, and the variable number is cut down to seven with this method. In general, once the coordinates and the radius of the three circles are confirmed, the angles of  $\alpha$  and  $\theta$  (see Fig. 1) can be determined. Thus, the point number and the coordinates of every single point on the piston bowl shape line can be determined, and the piston bowl geometry can be described.



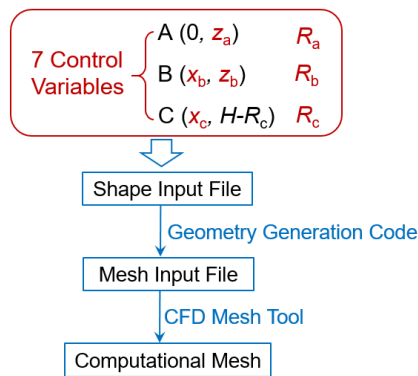
154 Fig. 1. Illustration of automatic generation of the piston bowl geometry.  
155  
156

157 The common piston bowl geometries widely used in previous studies for advanced combustion modes, including  
158 the Open, Re-entrant, and Shallow piston bowl geometries, can be established using this method, as shown in Fig. 2.  
159 Because the bowl shape is specifically determined by the size and location relationship of the three control circles, it  
160 can be flexibly controlled by the variables shown in Fig. 1 for the optimization of the bowl shape. Fig. 3 illustrates

161 the computational mesh generation process. In this study, the computational mesh is generated using the pre-  
 162 processing tool for mesh establishment in the KIVA code. The input file for the pre-processing program is integrated  
 163 with the geometry generation code according to the shape input file, which includes the information of the three  
 164 control circles (*i.e.*, circles A, B, and C). Among various generated meshes, the computational sector meshes of three  
 165 typical piston bowl geometries with the geometric compression ratio of 14.4 are shown in Fig. 2. It can be seen that  
 166 the computational sector meshes for the Open, Re-entrant, and Shallow piston bowls can be well generated.  
 167



168 Fig. 2. Common piston bowl types and corresponding computational meshes at top dead center.  
 169



170  
 171 Fig. 3. Computational mesh generation procedure.  
 172

173 **2.2. CFD Model**

174 The CFD calculation of this study was conducted using the open-source KIVA-3V code [28] for simulating the

175 engine working process. Based on the framework of KIVA-3V, several improvements and updates about the sub-  
 176 models have been performed. The turbulence model improved by Wang et al. [29] was used for modeling the in-  
 177 cylinder flow. The improved models were used for modeling the spray impingement [30] and liquid film evolution  
 178 processes [31]. Moreover, the quasi-dimensional model for describing the vaporization processes of fuel droplets [32]  
 179 and liquid films [33] was integrated. Meanwhile, the wall heat transfer model [34], droplet collision model [35], and  
 180 droplet breakup model [36] were also contained in this CFD code. For dealing with the fuel chemistry, the KIVA-3V  
 181 code was coupled with the CHEMKIN solver [37]. Furthermore, the skeletal chemical mechanism constructed by  
 182 Chang et al. [38] was used for predicting the ignition and combustion characteristics of the fuel blends. The diesel  
 183 and gasoline fuel were represented by *n*-heptane and *iso*-octane, respectively. It should be noted that the above models  
 184 have been validated based on numerous experimental data in the previous works, e.g., Refs. [39, 40].

185  
 186

Table 2. Engine specifications

Bore (mm)	110.0
Stroke (mm)	135.0
Connecting rod length (mm)	212.5
Original compression ratio	14.4:1
Swirl Ratio	2.3
Direct fuel injection system	Common rail
Number of nozzle holes	7
Spray angle (°)	75.0
Nozzle hole diameter (mm)	0.177

187

188 The computational model was validated ahead of the optimization study. Table 2 lists the detailed information  
 189 of the engine tested in this work. The validation was performed at a constant engine speed of 1200 rev/min with  
 190 different IMEP. Table 3 lists the basic conditions and the operating parameters of the validation cases. Table 4 lists  
 191 the the properties of the diesel and gasoline fuels tested in the experiment [15]. Fig. 4 illustrates the computational  
 192 mesh for the original DMDF combustion chamber, and the mesh is generated using the method mentioned above.  
 193 Fig. 5 illustrates the comparison of the simulated and experimental in-cylinder pressure and heat release rate (HRR)

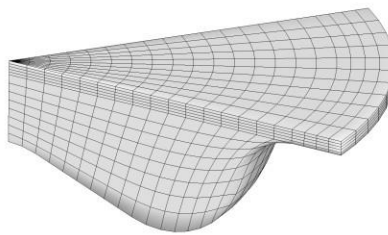
194 traces for five test cases with different IMEP. The comparison results show that the simulated traces can well match  
 195 with the measurements of Benajes et al. [15]. This indicates that the simulation with the generated computational  
 196 mesh can accurately reproduce the combustion process of the DMDF mode at different loads.

197  
 198 Table 3. Basic conditions of the validation cases.

IMEP (bar)	5.9	9.9	11.9	17.3	22.6
$p_{ivc}$ (bar)	1.60	2.29	2.32	3.01	3.09
$T_{ivc}$ (K)	332.6	329.1	347.9	332.2	356.1
EGR rate (%)	19.7	55.5	50.2	45.1	31.0
SOI1 (°CAATDC)	-48.0	-50.0	-45.0	-	-
SOI2 (°CAATDC)	-41.9	-4.4	-5.0	0.0	6.0
Total fuel flow (mg/cycle)	35.5	65.2	81.1	116.9	145.3
Diesel flow (mg/cycle)	31.8	62.3	50.4	52.9	49.3
Gasoline flow (mg/cycle)	3.7	2.9	30.7	64.0	96.0

199  
 200 Table 4. Properties of the diesel and gasoline fuels

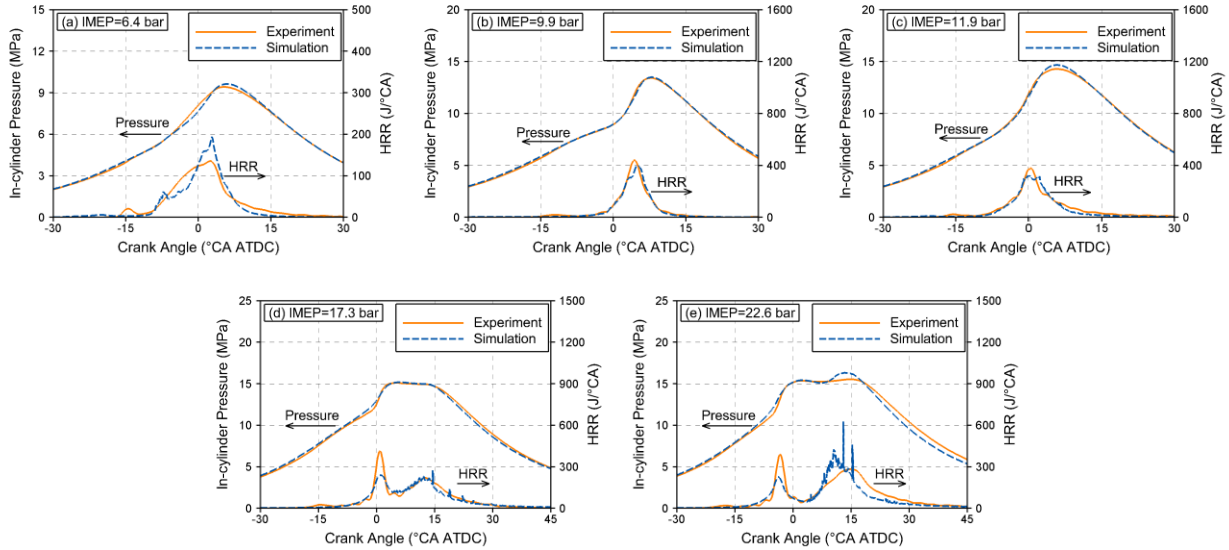
	Diesel	Gasoline
Density (kg/m <sup>3</sup> ) @ T=288.15 K	824	720
Viscosity (mm <sup>2</sup> /s) @ T=313.15 K	2.8	-
Research Octane Number (-)	-	95
Motor Octane Number (-)	-	85
Cetane Number (-)	51	-
Lower Heating Value (kJ/kg)	42.92	42.40



202  
 203 Fig. 4. Computational mesh for the original DMDF combustion chamber.  
 204

205 Fig. 6 shows comparisons of HC, CO, NO<sub>x</sub> and soot emissions between simulation and experiment. It is found  
 206 that the overall variation trend with varying IMEP can be well captured for the four emissions. However, the  
 207 discrepancies in magnitude still exist between the simulated and experimental emission levels. This is primarily  
 208 owing to the complexity of the in-cylinder flow and fuel/air mixing process, the imperfection of the chemical

209 mechanism [41], and the measurement uncertainties [3]. Since the main task of the simulation tool of this study can  
 210 be qualified by the capability of predicting the emission variation trend as a specific operating parameter changes,  
 211 the computational model and mesh can be employed for the optimization study in the following work.  
 212



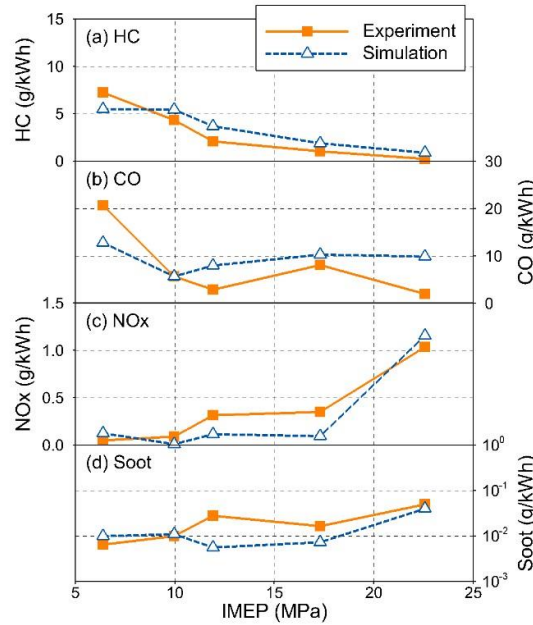
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Fig. 5. Validations of the pressure and HRR at different loads.



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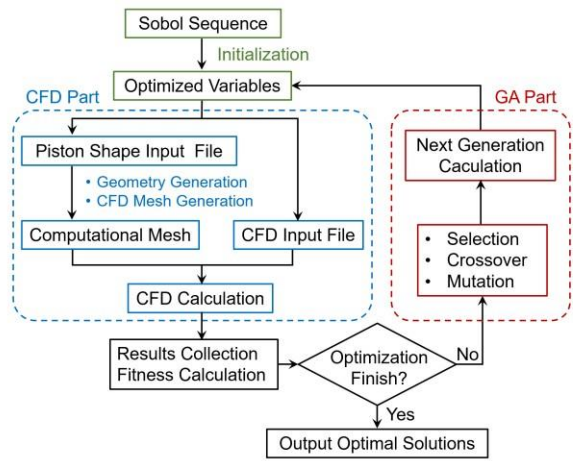
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Fig. 6. Validations of the emissions at different loads.

### 2.3. Optimization method

In this study, the optimization of the piston bowl geometry coupled with the injection strategy involves a

222 considerable number of variables. In order to realize the multi-variable multi-objective optimization and  
 223 simultaneously minimize the fuel consumption and engine-out emissions, the non-dominated sorting genetic  
 224 algorithm II (NSGA-II) [42] was utilized. The flowchart of the optimization procedure is illustrated in Fig. 7. The  
 225 global numerical system contains two parts, *i.e.*, the optimization part using GA and the CFD part using KIVA. The  
 226 GA code is coupled with the KIVA code containing the geometry generation code. In the optimization calculation,  
 227 the GA code generates the shape input and CFD input files. The geometry generation code is in charge of exporting  
 228 the mesh input file, which is the input file for the meshing program to create the computational mesh. CFD calculation  
 229 is performed with the CFD input file and the computational mesh. GA code analyzes the CFD calculation results of  
 230 each citizen and generates new data for the next generation calculation.

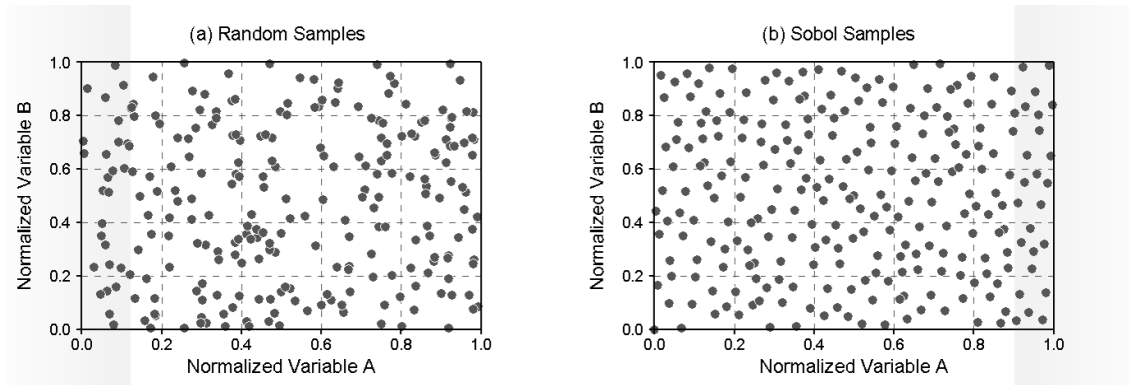


231  
 232 Fig. 7. Illustration of the optimization computation process.  
 233

234 Considering the increased number of variables, the initial population size needs to be enlarged to keep the  
 235 diversity of the optimal solutions in the GA calculation. In this study, the initialization of the citizens for the first  
 236 generation is improved by introducing the Sobol sequence sampling method [43] instead of the traditional random  
 237 sampling method used in NSGA-II. Fig. 8 shows the distributions of the random samples and Sobol samples with a  
 238 constant sample number of 250 in a two-dimensional variable coordinate. It can be found that the distribution of the  
 239 Sobol samples is more uniform than that of the random samples. This indicates that the Sobol sequence sampling



240 method can provide a better uniformity for the multi-dimensional variables by sufficiently covering the whole  
241 variation ranges of the variables under the conditions with limited population size. Therefore, the introduction of the  
242 Sobol sequence sampling method in this study is aiming at including more possible cases and searching for the global  
243 optimal solutions more effectively, and a relatively small population size can be utilized simultaneously for saving  
244 computational resources.  
245



246

247

248

Fig. 8. Comparison of random samples and Sobol samples.

### 249 3. Results and Discussion

#### 250 3.1. Global optimization results

251 In a previous study from the authors [19], based on the diesel/gasoline DMDF combustion concept, the operating  
252 parameters related to the injection strategy and the air intake conditions were optimized to enhance the engine  
253 performance (*i.e.*, Step 1 optimization). A total of seven operating parameters with crucial influences were chosen as  
254 the variables at three different loads in the previous study. Since the injection/wall interaction plays a critical role in  
255 the fuel/air mixture formation, the optimization of the injection parameters cooperated with the piston bowl geometry  
256 was further conducted at different load conditions in this study (*i.e.*, Step 2 optimization). The aim is to search for  
257 the most suitable piston bowl shape for the DMDF combustion mode over a wide load range. A total of 14 parameters  
258 were considered in the present work, including seven geometric parameters and seven engine operating parameters.  
259 The optimization specifications are listed in Table 5.

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Table 5. Optimization specifications

	Parameter	Range
Variables	Premix Ratio	(0.0, 1.0)
	SOI1 (°CA ATDC)	(-80.0, 10.0)
	SOI2 (°CA ATDC)	(SOI1, 10.0)
	MF1	(0.0, 1.0)
	Spray angle (°)	(15, 85)
	Injection Pressure (MPa)	(50, 180)
	Compression Ratio	(12.0, 18.0)
	Normalized $Z_a$	(0.0, 1.0)
	Normalized $Z_b$	(0.0, 1.0)
	Normalized $X_b$	(0.0, 1.0)
	Normalized $X_c$	(0.0, 1.0)
	Normalized $R_a$	(0.0, 1.0)
	Normalized $R_b$	(0.0, 1.0)
Normalized $R_c$	(0.0, 1.0)	
Constraints	EISFC (g/kWh)	<250.0
	$T_{max}$ (K)	>1100.0
	NO <sub>x</sub> (g/kWh)	<0.4
	soot (g/kWh)	<0.01
	PPRR (bar/°CA)	<15.0
	$p_{max}$ (MPa)	<20.0
	RI (MW/m <sup>2</sup> )	<10.0

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Table 6. Initial conditions at IVC timing at each load.

	Low	Mid	High
$p_{ivc}$ (bar)	1.51	1.99	3.30
$T_{ivc}$ (K)	392.2	306.1	315.5
EGR (%)	6.5	6.5	31.0

264

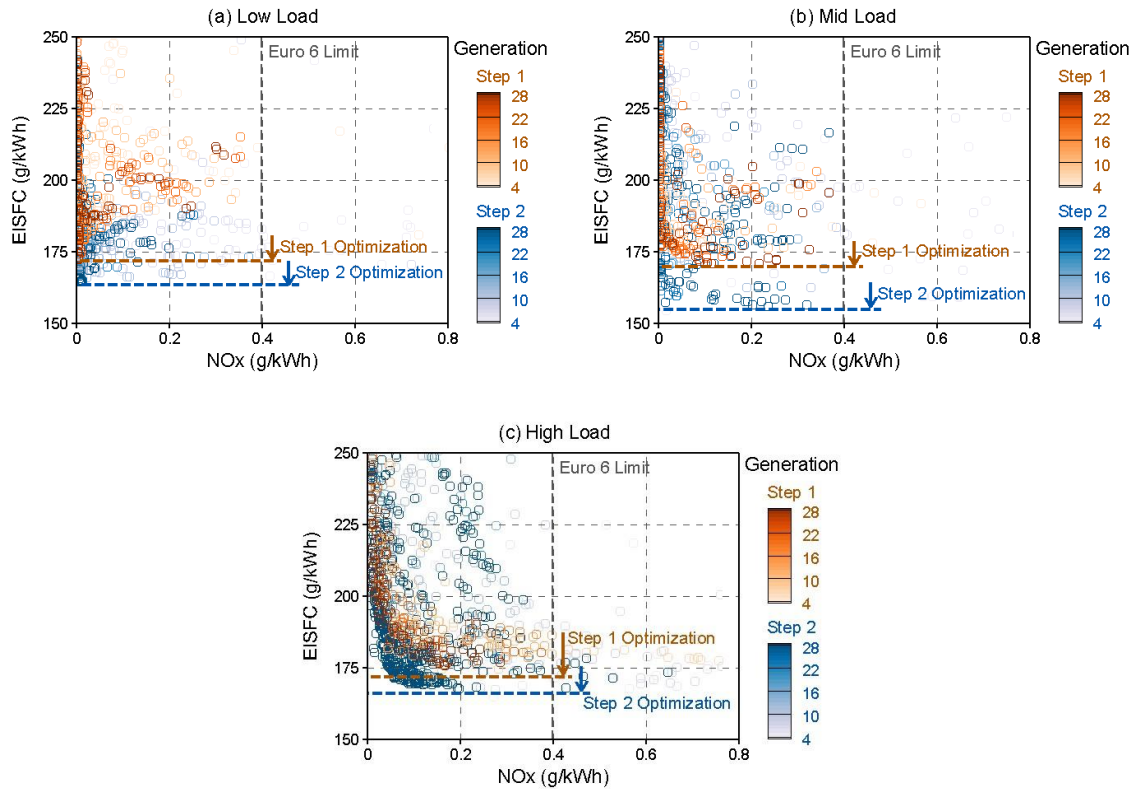
265 The seven geometric parameters are normalized  $Z_a$ ,  $Z_b$ ,  $X_b$ ,  $X_c$ ,  $R_a$ ,  $R_b$ , and  $R_c$ , which determine the piston bowl  
266 shape, as illustrated in Figs. 1 and 2. The variation ranges of the geometric parameters are all from 0.0 to 1.0. The  
267 operating parameters relating to the direct fuel injection event include the two injection timings (*i.e.*, SOI1 and SOI2),  
268 injection pressure (*i.e.*,  $p_{inj}$ ), mass fraction of the first injection (*i.e.*, MF1), and spray angle (SA). The variation ranges  
269 of the injection parameters can be found in Table 5. The SA is equal to a half of the injection plume included angle.  
270 Moreover, the premix ratio (*i.e.*, PR) of gasoline fuel and geometric compression ratio (*i.e.*, GCR) were also included  
271 in the variables to be optimized. In the engine simulations, the squish height was adjusted to match the desired GCR.

272 During the optimization process, the equivalent indicated specific fuel consumption (EISFC), NO<sub>x</sub>, and soot  
273 emissions are selected as the objectives to urge the populations into the pleasant fuel economy and low-emission  
274 orientation. Meanwhile, several constraints are taken into consideration in order to guarantee the rationality of the  
275 optimal cases. In the optimization calculation, the peak in-cylinder temperature is kept above 1100 K to avoid misfire.  
276 For forbidding rough engine operations, the maximum in-cylinder pressure ( $p_{\max}$ ), ringing intensity (RI), and PPRR  
277 are limited under 19.0 MPa, 10 MW/m<sup>2</sup>, and 15.0 bar/°CA, respectively [15]. The EISFC is restricted under 250  
278 g/kWh to ensure satisfactory fuel economy, while the NO<sub>x</sub> and soot emission limits are set according to the Euro VI  
279 regulations (*i.e.*, 0.4 and 0.01 g/kWh, respectively). Moreover, the operating loads for optimization are located at 5.9,  
280 11.9, and 22.6 bar, which are chosen from the baseline cases validated in Section 2.2. According to our previous  
281 study, the optimized air intake conditions including the initial temperature ( $T_{\text{ivc}}$ ) and pressure ( $p_{\text{ivc}}$ ) at IVC timing, as  
282 well as the EGR rate, are used in this work. Table 6 lists the setup of the initial conditions at the IVC timing for the  
283 optimization calculation at the three loads.

284 The optimization results of the present study are first compared with the previous optimization results to  
285 demonstrate the improvements gained from the piston bowl geometry optimization. Fig. 9 shows the evolution of the  
286 EISFC and NO<sub>x</sub> emissions for all the generated cases in the population at the various loads. The yellow and blue  
287 symbols represent the generated cases in the previous optimization (*i.e.*, Step 1 optimization) and the present  
288 optimization (*i.e.*, Step 2 optimization), respectively. Each case is colored by the generation number. A deeper color  
289 denotes a higher optimization degree. From the comparison of the Step 1 optimization to the Step 2 optimization, it  
290 can be found that EISFC is further decreased after the piston bowl geometry optimization while NO<sub>x</sub> emissions can  
291 still meet the Euro VI limit. The soot emissions of the optimal cases (*i.e.*, the deeper-color symbols) are also below  
292 the Euro VI limit, which is not illustrated in Fig. 9 due to space limitation. This well demonstrates the improvement  
293 of fuel economy without sacrificing the engine-out emissions in the Step 2 optimization. Overall, the above results

294 indicate that the piston bowl geometry optimization further enhances the performance of the DMDF combustion  
295 mode at different loads.

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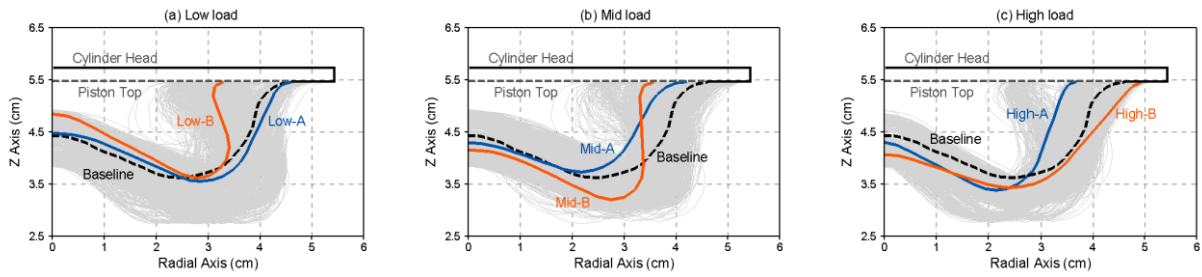
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299 Fig. 9. Evolution of the EISFC and NO<sub>x</sub> emissions during the optimization at different loads.

300

301 Fig. 10 shows the comparison of the piston bowl shapes obtained during the optimization process at different  
302 loads. The dashed black line represents the baseline piston bowl shape for the DMDF mode [15]. The dashed grey  
303 line represents the top dead center position. The solid grey lines denote all the piston bowl profiles generated from  
304 the genetic algorithm. In this section, the cases with competitive fuel efficiency while meeting the Euro VI standards  
305 of the NO<sub>x</sub> and soot emissions are chosen as the optimal cases at each load. Furthermore, in order to provide more  
306 options for the DMDF piston bowl geometry design, among the optimal piston bowls, two typical shapes with  
307 distinguishing geometric characteristics are picked up to represent the optimal piston geometry at each load. The  
308 selected optimal cases are named as Low-A and Low-B for low load, Mid-A and Mid-B for mid load, and High-A  
309 and High-B for high load. As shown in Fig. 10, the optimal shapes are represented by the orange and blue lines.

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Fig. 10 Generated piston bowl shapes and typical optimal piston bowl shapes in the optimization at different loads.

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It is seen from Fig. 10 that the optimal bowl geometries at low and mid loads contain both the open type and re-entrant type bowl, whereas the high load only contains the open type bowl. At low load, the optimal re-entrant type bowl (*i.e.*, case Low-B) features a smaller bowl width, while the optimal open type piston bowl (*i.e.*, case Low-A) features a similar bowl width compared with the baseline piston bowl, as shown in Fig. 10(a). At mid load, the optimal open type piston bowl (*i.e.*, case Mid-A) characterizes a relatively larger bowl width and smaller bowl depth, while the optimal re-entrant type bowl (*i.e.*, case Mid-B) characterizes a relatively smaller bowl width and larger bowl depth, as shown in Fig. 10(b). At high load, the two optimal cases feature a smaller bowl width (*i.e.*, case High-A) and a larger bowl width (*i.e.*, case High-B), respectively. Meanwhile, both of the two optimal cases at high load exhibit larger bowl depth compared with the baseline piston geometry, as shown in Fig. 10(c).

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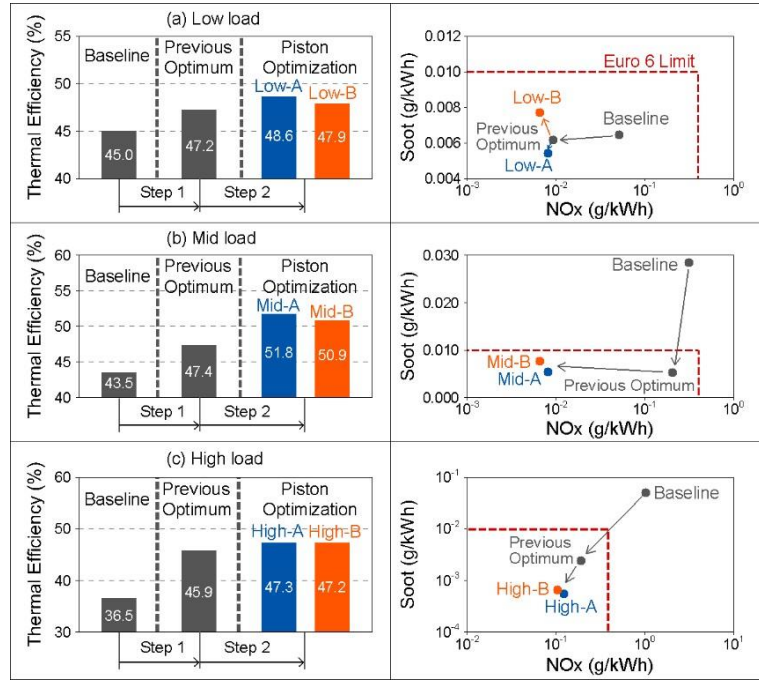
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330

In order to demonstrate the engine improvements using the optimal piston bowl shapes, the optimal cases are compared to the previous optimal cases and the baseline cases in terms of fuel efficiency,  $\text{NO}_x$  and soot emissions, as shown in Fig. 11. The grey bars and symbols represent the baseline cases and the optimal cases from the previous optimization (*i.e.*, Step 1 optimization). The orange and blue bars and symbols represent the optimal cases from the piston bowl geometry optimization (*i.e.*, Step 2 optimization). The left figures illustrate the comparisons of thermal efficiency, and the right figures provide the comparisons for  $\text{NO}_x$  and soot emissions. As depicted in the left sub-figures of Fig. 11, significant improvement can be found for the thermal efficiency with the previous optimization (*i.e.*, Step 1) at the three loads. After optimizing the piston bowl shape combined with the injection parameters (*i.e.*,

331 Step 2), the thermal efficiency is further improved. The thermal efficiency is increased up to 1.4%, 4.4%, and 1.4%  
 332 for the low, mid, and high loads, respectively. It is worth noting that an indicated thermal efficiency up to 51.8% can  
 333 be realized at mid load with the combined optimization. This well demonstrates the benefit gained for fuel economy  
 334 from the piston bowl geometry optimization.

335



336

337 Fig. 11. Comparisons of thermal efficiency, NO<sub>x</sub> emissions, and soot emissions among the baseline cases and the  
 338 optimal cases in Step 1 and Step 2 optimizations.  
 339

340 As for the right sub-figures of Fig. 11, both the NO<sub>x</sub> and soot emissions are continuously decreased after Step 1  
 341 and Step 2 optimizations at high load. At low and mid loads, the improvements of NO<sub>x</sub> and soot emissions for Step  
 342 2 optimization are not as significant as those for Step 1 optimization, but either NO<sub>x</sub> or soot emissions can still be  
 343 further decreased to some extent after Step 2 optimization compared to the cases of Step 1 optimization. For both the  
 344 optimal cases, the NO<sub>x</sub> and soot emissions can meet the Euro VI limits. Thus, it is concluded that the thermal  
 345 efficiency can be significantly improved with the piston bowl geometry optimization without sacrificing NO<sub>x</sub> and  
 346 soot emissions.

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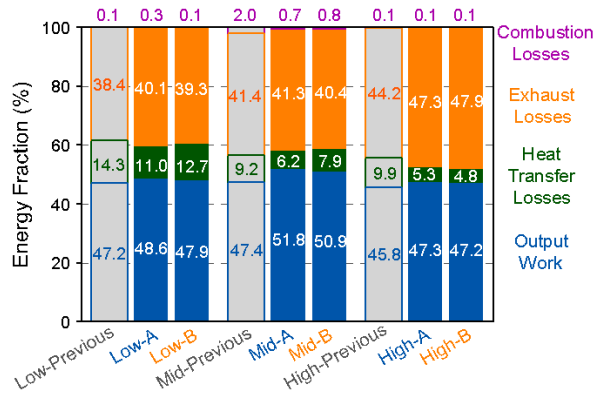


Fig. 12. Illustration of the energy fractions of optimal cases and baseline cases.

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Furthermore, the energy analysis was conducted for investigating fuel efficiency benefits. As illustrated in Fig.

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12, the energy fractions of the optimal cases in Step 2 optimization are compared with those of the previous optimal

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cases in Step 1 optimization. The bar colored by grey represents the previous optimal case while the other two

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represent the optimal cases from the piston bowl geometry optimization at each load. According to the first law of

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thermodynamics, the total input fuel energy is transferred into four parts during the combustion process, including

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output work, heat transfer losses, exhaust losses, and incomplete combustion (*i.e.*, combustion losses), as shown in

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Fig. 12. It is noted that the energy fraction of output work is directly related to the thermal efficiency depicted in Fig.

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11. It can be seen from Fig. 12 that the purple bars are not obviously visible, which is due to the fact that the

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combustion losses are relatively low (less than 1%) under the whole load range. This is because that a majority of

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HC and CO emissions are reduced by the oxidation reactions in the late combustion stage. Thus, the engine-out

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emission levels of HC and CO are low. From the comparison of the optimal cases from the piston bowl geometry

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optimization with those from the previous optimization, it can be found that the improvement of the output work (*i.e.*,

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thermal efficiency) is mainly resulted from the decrease of the heat transfer losses at low and high loads. At mid load,

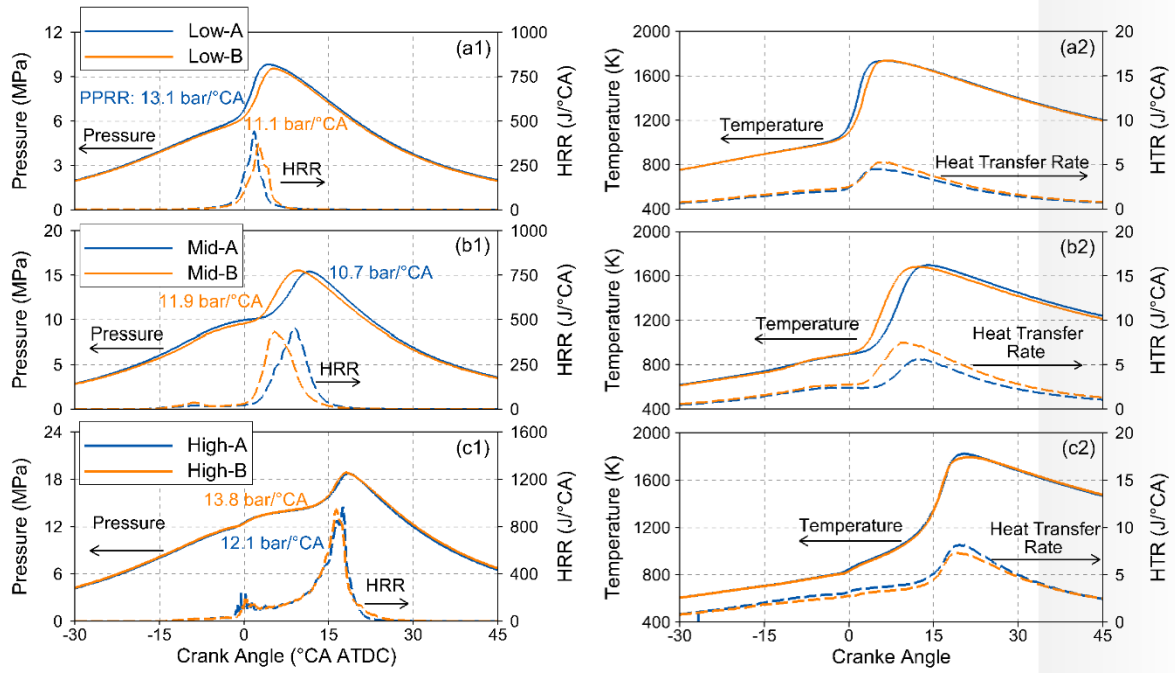
364

the decreases of both the heat transfer losses and combustion losses contribute to the improvement of output work.

365

This demonstrates the benefits of thermal efficiency gained from the piston bowl geometry optimization.

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Fig. 13. Comparison of the in-cylinder pressure, HRR, temperature, and heat transfer rate (HTR) traces between the optimal cases.

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Furthermore, the combustion process of the optimal cases is analyzed in detail for further explaining the

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improved performance after the piston bowl geometry optimization. Fig. 13 depicts the in-cylinder pressure,

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temperature, HRR, and heat transfer rate (HTR) traces of the optimal cases. Overall, from the comparisons of the

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pressure, temperature, and HRR, it is found that the traces at each load are very similar, especially for the high load

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condition, in spite of slight differences existing in the combustion phasing between the different optimal cases. This

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indicates that the different optimal cases exhibits similar combustion characteristics at each load. In terms of the

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comparison of the three loads, the combustion phasing is found to be retarded with increasing load, which is

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consistent with previous results [11, 19]. This is mainly aiming at controlling ringing intensity and preventing the

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engine knock. It can be seen from the denoted PPRR in Fig. 13 that at mid and high loads, by managing the

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combustion process and combustion phasing, the PPRR can meet the limit of 15 bar/°CA. At low load, although a

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relatively advanced combustion phasing is presented, the PPRR is still under the limit since the released fuel energy

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is much lower than those of mid and high loads.



383 Moreover, in order to understand the heat transfer process, the heat transfer rate (HTR) traces of the optimal  
 384 cases at each load are also illustrated in Fig. 13. By comparing the HTR traces at each load, the differences in the  
 385 heat transfer losses (see Fig. 12) can be explained. It can be found that the global HTR of cases Low-B, Mid-B, and  
 386 High-A is higher than that of cases Low-A, Mid-A, and High-B, respectively. Thus, the heat transfer losses of cases  
 387 Low-B, Mid-B, and High-A are relatively higher. However, the heat transfer process cannot be simply explained by  
 388 the evolution of the global in-cylinder temperature since the piston bowl geometry and the combustion occurrence  
 389 location also play critical roles. Thus, this will be explained in the following section.

### 390 3.2. Typical optimal piston bowl geometry and corresponding injection strategy

392 In this section, the optimal piston bowl shape coupled with the corresponding fuel injection strategy is  
 393 summarized at each load. Table 7 lists the operating parameters of each optimal cases. Meanwhile, the fuel injection  
 394 event and the fuel/air mixture formation process are analyzed as well. Fig. 14 shows the liquid fuel distribution after  
 395 injection timing and the equivalence ratio distribution before ignition for cases Low-A and Low-B. As mentioned  
 396 above, the optimal bowl shape for case Low-A is open type, while the optimal bowl shape for case Low-B is re-  
 397 entrant type. Besides, as listed in Table 7, both of the two optimal cases utilize a similar compression ratio with that  
 398 of the original engine setup (*i.e.*, 14.4) [15].

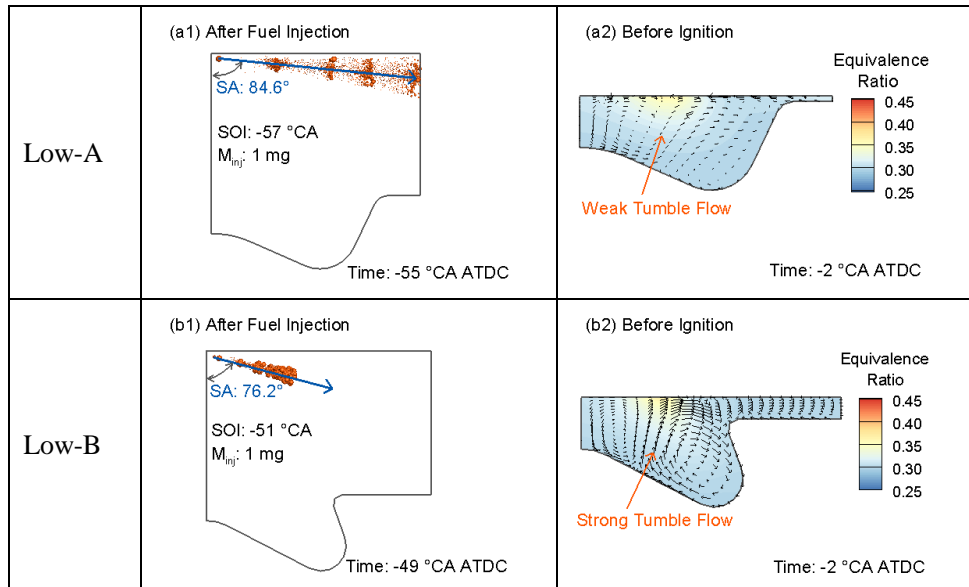
399 Table 7. Operating parameters of the optimal cases.

	Low-A	Low-B	Mid-A	Mid-B	High-A	High-B
CR	14.6	14.7	16.7	15.8	14.0	13.8
PR	97%	97%	90%	76%	96%	96%
$p_{inj}$ (MPa)	167	101	140	162	176	175
SOI1 (°CA ATDC)	-57	-51	-56	-79	-28	-26
SOI2 (°CA ATDC)	-	-	-51	-60	-15	-18

401  
 402 As for the fuel injection strategy, only the cases with the single injection strategy are retained in the genetic  
 403 algorithm optimization at low load. By comparing Figs. 14(a1) and 14(b1), it is found that case Low-A is coupled

404 with a relatively wider spray angle (SA) of  $84.6^\circ$ . In contrast with case Low-A, case Low-B is coupled with a  
 405 relatively narrower SA of  $76.2^\circ$ , which is similar to that of the original experimental setup (*i.e.*,  $75^\circ$ ) [15]. Figs. 14(a2)  
 406 and 14(b2) illustrate the in-cylinder equivalence ratio distributions before ignition for cases Low-A and Low-B,  
 407 respectively. From the comparison, it can be found that the high fuel concentration locations of the two cases are  
 408 similar, which is owing to the combined effects of the piston bowl geometry and the fuel injection event. As can be  
 409 seen, a stronger tumble flow is organized in the re-entrant piston bowl geometry in contrast to the open type bowl,  
 410 which is also indicated by Miles and Andersson [44], as well as Lee et al. [45]. This results in larger flow velocity  
 411 around the cylinder head and the piston wall near top dead center (TDC) for case Low-B. Thus, although a relatively  
 412 lower injection pressure ( $p_{inj}$ ) and a later SOI timing are employed for case Low-B, the injected fuel can also  
 413 propagate to the similar location as that of case Low-A.

414



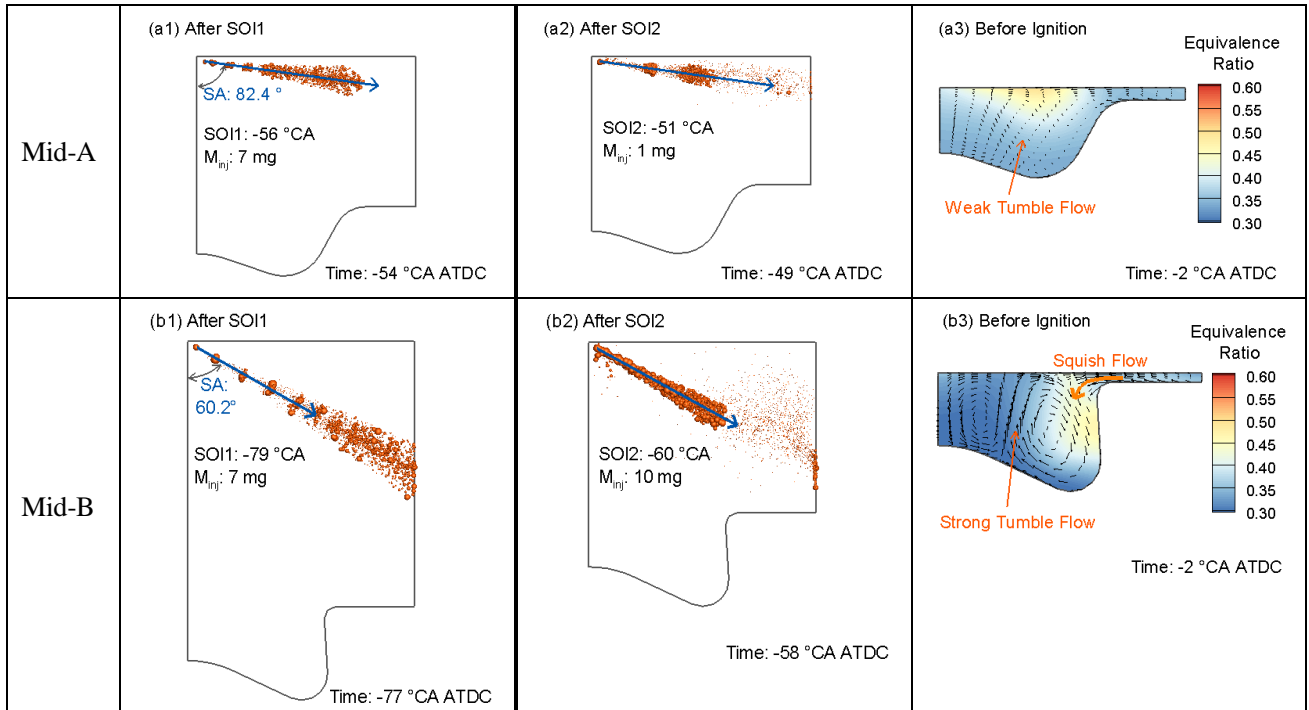
415 Fig. 14. Illustration of the optimal piston bowl shape, fuel injection and the fuel/air mixture formation at low load.

416

417 Fig. 15 depicts the liquid fuel distribution after injection timing and the equivalence ratio distribution before  
 418 ignition for the optimal cases at mid load (*i.e.*, cases Mid-A and Mid-B). The shallow open piston bowl of case Mid-  
 419 A is coupled with a relatively wider SA and lower injection pressure, as well as later fuel injection timings. On the  
 420 contrary, the deep re-entrant piston bowl of case Mid-B is integrated with a relatively narrower SA and higher

421 injection pressure, as well as earlier fuel injection timings. For case Mid-A, due to the lower  $p_{inj}$  and wider SA  
 422 compared to that of case Mid-B, the fuel spray penetration is relatively shorter, and the fuel mainly concentrates near  
 423 the cylinder head, as shown in Fig. 15(a3), which is similar to the situation at low load. For case Mid-B, owing to the  
 424 higher  $p_{inj}$  and earlier fuel injection timings, the fuel penetration spray is much longer, which takes more fuel into the  
 425 squish region. However, the strong squish flow in case Mid-B brings most of the injected fuel back into the bowl  
 426 region, as shown in Fig. 15(b3). Meanwhile, the strong tumble flow resulted from the deep piston bowl geometry is  
 427 helpful for the fuel/air mixing in case Mid-B with the employment of more injected fuel. Furthermore, as listed in  
 428 Table 4, relatively higher CRs are employed in cases Mid-A and Mid-B for strengthening fuel efficiency. Thus, a  
 429 significant improvement in thermal efficiency can be seen in Fig. 11. Meanwhile, with the help of lower initial  
 430 temperature (see Table 3), the combustion phasing can be well controlled and the PPRR limit is maintained at mid  
 431 load.

432



433 Fig. 15. Illustration of the optimal piston bowl shape, fuel injection and the fuel/air mixture formation at mid load.

434

435 As for high load, as shown in Fig. 16, both cases High-A and High-B employ the open type piston bowl. The

436 difference is that case High-A utilizes a deep-narrow bowl geometry, while case High-B employs a shallow-wide

437 open bowl geometry. Moreover, case High-A is coupled with a narrower SA, whereas case High-B uses a wider SA.

438 In terms of fuel injection timings, both of the SOI1 and SOI2 timings of cases High-A and High-B are retarded

439 compared with those of the optimal cases at low and mid loads. This is for avoiding advanced ignition, which can

440 lead to high pressure rise rate and consequently engine knock at high load. Meanwhile, the relatively lower

441 compression ratio employed by cases High-A and High-B (see Table 4) is also beneficial for controlling the PPRR.

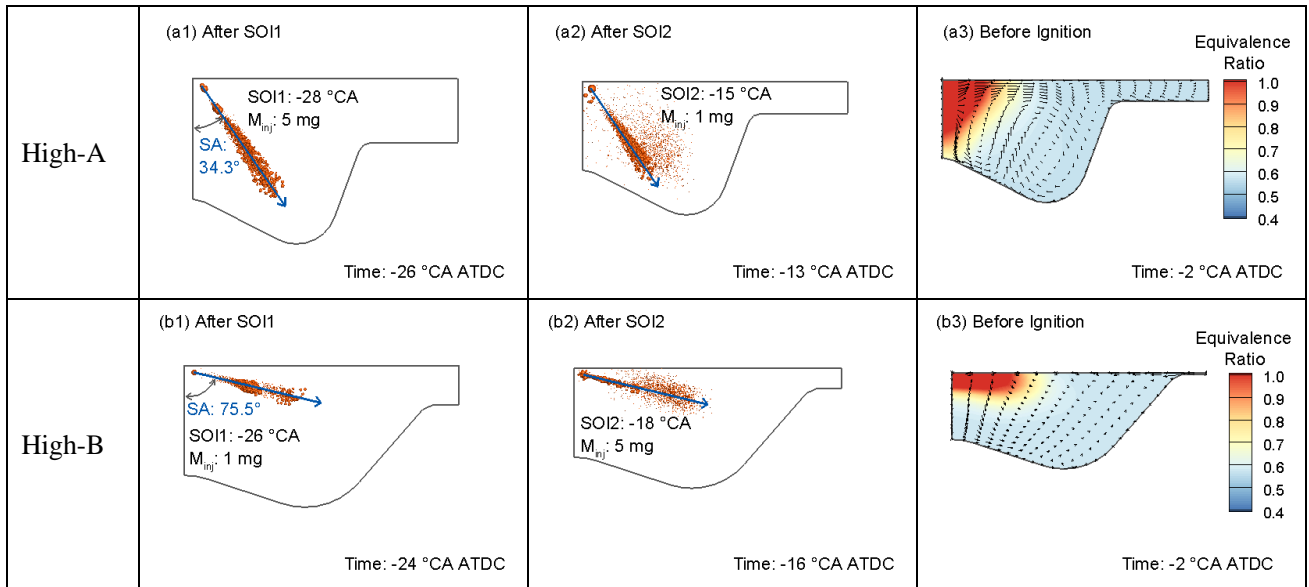
442 In such a way, a large fraction of gasoline can be premixed for the DMDF combustion mode at high load without

443 exceeding the PPRR limit. Therefore, as shown in Table 4, the premix ratio of cases High-A and High-B can be

444 increased to an equivalent level as that of mid and low loads. This is helpful for controlling the  $\text{NO}_x$  and soot

445 emissions owing to the premixed combustion enhancement.

446



447 Fig. 16. Illustration of the optimal piston bowl shape, fuel injection and the fuel/air mixture formation at high load.

448

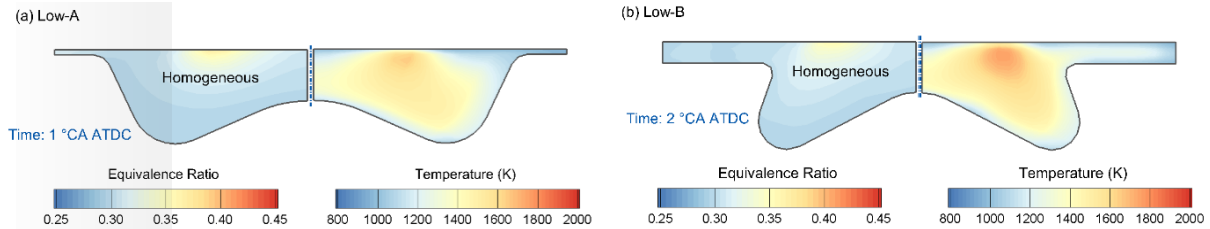
449 The late injection timings combined with the less injected fuel mass result in shorter fuel penetrations for cases

450 High-A and High-B. Moreover, although the injection pressure is higher than lower loads (see Table 4), the increasing

451 in-cylinder charge density resulted from the higher intake pressure at high load (see Table 3) restricts the propagation

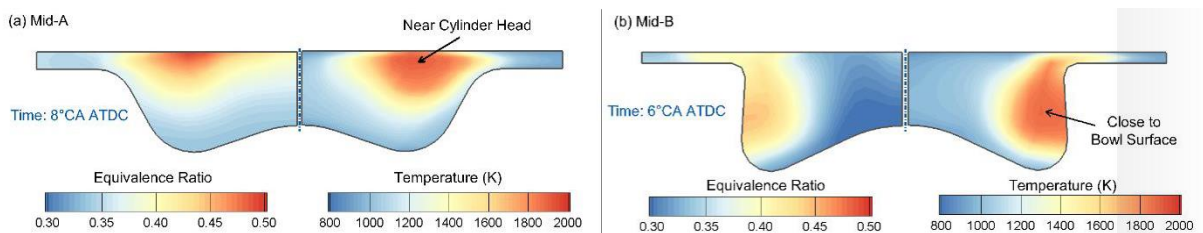
452 of the injected diesel fuel. Thus, the injected fuel mainly concentrates around the injection nozzle region, as shown

453 in Figs. 16(a3) and 16(b3). Furthermore, from the comparison of the flow field of cases High-A and High-B, it is  
 454 confirmed again that the deep and narrow bowl geometry can produce strong tumble flow compared with the shallow  
 455 and wide piston geometry.



457  
 458 Fig. 17. In-cylinder equivalence ratio and temperature distributions at CA50 for cases Low-A and Low-B.  
 459

460 In order to further investigate the combustion characteristics of the optimal cases, the in-cylinder temperature  
 461 and equivalence ratio distributions during the combustion process are further analyzed in this section. Figs. 17 to 19  
 462 depicts the in-cylinder temperature and equivalence ratio distributions at the time of 50% burning point (CA50) for  
 463 the optimal cases of low, mid, and high loads, respectively. It can be found that the locations of the high fuel vapor  
 464 concentration and the combustion occurrence are directly related to the fuel distribution pattern before ignition shown  
 465 in the above figures, which is determined by the joint effects of piston bowl geometry and fuel injection strategy. As  
 466 shown in Fig. 17, since the direct-injected fuel mass is lower, and a majority of fuel is premixed in the intake port,  
 467 both cases Low-A and Low-B exhibit a homogeneous equivalence ratio distribution. This leads to the corresponding  
 468 homogeneous combustion characteristics for both the optimal cases, which is helpful for the NO<sub>x</sub> and soot emission  
 469 control. This is consistent with the previous results at low load operation [19].

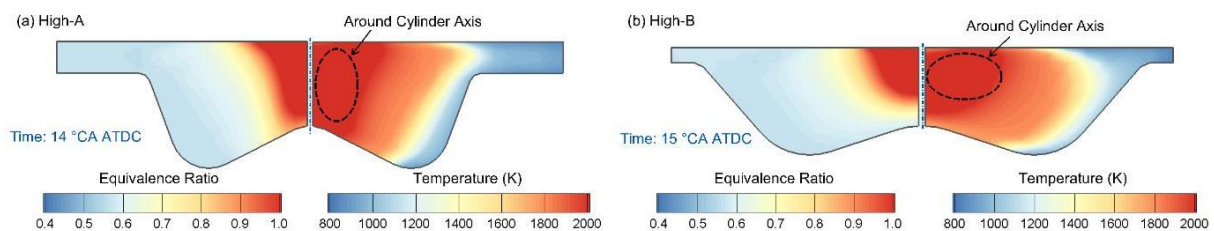


471  
 472 Fig. 18. In-cylinder equivalence ratio and temperature distributions at CA50 for cases Mid-A and Mid-B.  
 473

474 At mid load, with the increase of the injected fuel mass, the local equivalence ratio concentration is increased  
 475 compared with the low load, as seen in Fig. 18. For case Mid-A, consistently with the low-load optimal cases, a high  
 476 premix ratio (see Table 4) is utilized for enhancing the premix combustion, leading to pleasant NO<sub>x</sub> and soot  
 477 emissions. For case Mid-B, although a higher direct-injected diesel fuel mass (*i.e.*, lower premix ratio) is employed,  
 478 the local equivalence ratio concentration is lower than that of case Mid-A. This is because that the optimized deep  
 479 re-entrant piston bowl geometry of case Mid-B produces a stronger tumble flow within the bowl region, leading to  
 480 more sufficient premixing of the injected fuel with the in-cylinder charge before the combustion occurs. Thus, the  
 481 Euro VI emission limits for the NO<sub>x</sub> and soot emissions can also be maintained for case Mid-B. Moreover, consistent  
 482 with the vapor distribution of the direct-injected diesel fuel before ignition (see Fig. 15), the combustion occurrence  
 483 location is near the cylinder head and close to the bowl surface for case Mid-A and case Mid-B, respectively.

484 At high load, although the injected mass is not further increased, the local equivalence ratio concentration is  
 485 considerably elevated for the optimal cases, as illustrated in Fig. 19. This is mainly due to the shorter fuel spray  
 486 penetration resulted from the later fuel injection timing and the increased in-cylinder charge density. Correspondingly,  
 487 the combustion occurs near the cylinder axis region, which places the high-temperature region away from the piston  
 488 bowl surface or the cylinder wall during the combustion phasing.

489



490

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Fig. 19. In-cylinder equivalence ratio and temperature distributions at CA50 for cases High-A and High-B.

492

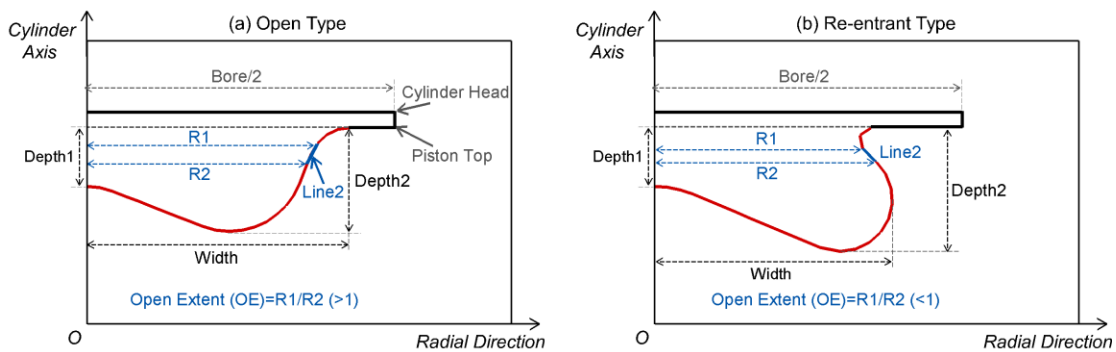
493 Moreover, the differences existing in the energy fraction of the heat transfer losses (see Fig. 12) between the  
 494 optimal cases at each load can be further explained in this section. At low load, it is easy to find that the re-entrant  
 495 type bowl of case Low-B exhibits a larger surface area compared with the open type bowl. Thus, although there is

496 no obvious difference in the combustion temperature between cases Low-A and Low-B, the heat transfer energy  
497 fraction of case Low-B is higher than that of case Low-A due to the larger heat transfer area. Similarly, at mid load,  
498 the deep re-entrant piston bowl of case Mid-B yields a larger heat transfer surface. Meanwhile, for case Mid-B, the  
499 high-temperature region is closer to the bowl surface. Therefore, the heat transfer energy fraction is higher for case  
500 Mid-B than case Mid-A. At high load, as mentioned above, the high-temperature regions are away from the bowl  
501 surface for both the two optimal cases. This is beneficial for reducing heat transfer losses. Moreover, although the  
502 two optimal cases at high load employ the open type piston bowl, the heat transfer surface area of case High-B is  
503 smaller due to the opener and wider bowl geometry. Thus, the heat transfer energy fraction of case High-B is slightly  
504 higher than that of case High-A (see Fig. 12).

### 505 506 3.3. Correlation analysis

507 From the above discussion, it can be summarized that the in-cylinder fuel/air mixture formation and combustion  
508 processes are affected by the piston bowl geometry and the fuel injection strategy simultaneously. Thus, the  
509 performance of the DMDF combustion mode directly depends on the combined effects of the geometric parameters  
510 and the fuel injection parameters. For further understanding the influences of these parameters on the DMDF  
511 combustion mode, a correlation analysis was conducted to investigate the sensitivity of the engine performance to  
512 the various parameters at each load in this section. It is noted that 14 parameters were considered as the optimization  
513 variables in this study, which results in the significant complexity of the correlation analysis. Fortunately, a large  
514 number of cases (*i.e.*, citizens) were generated in the GA calculation process. In addition, with the introduction of the  
515 Sobol sequence sampling method for GA in this study, the distribution uniformity for the multi-dimensional variables  
516 of the numerous cases can be ensured, which provides a high-quality database for the correlation analysis in this  
517 section. The aim of the correlation analysis is to investigate the influence weight of each input parameter to the  
518 performance parameter including emissions for the DMDF concept.

519 Before the correlation analysis, the seven geometric parameters (see Fig. 3) were cut down and transferred into  
520 four key parameters for simplifying the analysis complexity. Fig. 20 depicts the definitions of the four new geometric  
521 parameters, including Depth1, Depth2, Width, and Open Extent (OE). The variable of Width is defined as the distance  
522 from the cylinder axis to the right edge of the piston bowl. Moreover, as indicated in Fig. 1, the piston bowl profile  
523 consists of two lines and three circle curves. The type of the piston bowl is directly determined by the orientation of  
524 Line2. Thus, in this section, a new parameter, *i.e.*, Open Extent, is introduced to describe the piston bowl type. The  
525 definition of Open Extent can be found in Fig. 20, which is equal to the ratio of R1 to R2 where R1 and R2 are the  
526 distances from the cylinder axis to the endpoints of Line2. Overall, the four new geometric parameters can well reflect  
527 the piston bowl characteristics.  
528



529  
530 Fig. 20. Illustration of the key parameters for describing the bowl geometry of different types.  
531

532 Subsequently, the correlation analysis was conducted between the input parameters and the performance  
533 parameters. The input parameters contain the four new geometric parameters and five injection parameters, including  
534 the SOI1, SOI2, MF1, SA, and  $p_{inj}$ . The performance parameters contain the energy fractions of heat transfer losses  
535 (HTL) and combustion losses (CL), as well as the  $NO_x$  and soot emissions, which can reflect the combustion and  
536 emission characteristics of the DMDF engine. In this study, the correlation analysis is performed based on the  
537 Spearman Rank Correlation (SRC) coefficient [46]. This method is capable of providing the statistical relevance  
538 between the model input parameters and the target output parameters, and it has been widely used in engineering



539 applications [47-49]. The SRC coefficient is defined as

$$540 \quad \text{SRC} = \frac{\text{COV}(R_x, R_y)}{\sigma_{R_x} \sigma_{R_y}} \quad (1)$$

541 where  $x$  and  $y$  respectively represent the input and target output parameters,  $R_x$  and  $R_y$  respectively denote the rank

542 values of parameters  $x$  and  $y$ ,  $\text{COV}(R_x, R_y)$  is the covariance of  $R_x$  and  $R_y$ , and  $\sigma_{R_x}$  and  $\sigma_{R_y}$  represent the standard  
543 deviations of  $R_x$  and  $R_y$ . In this study, the samples are chosen from the citizens generated in the GA calculation. After

544 excluding the unreasonable cases with deteriorated combustion efficiency or rough engine operations, around 500  
545 effective cases are retained as the samples for the correlation analysis at each load.

546 Figs. 21 to 23 illustrate the SRC coefficient of each input parameter to each performance parameter at low, mid,  
547 and high loads, respectively. In each figure, the left and right parts depict the SRC coefficient of the geometric  
548 parameters and the injection parameters, respectively. The range of the SRC coefficient is from  $-1.0$  to  $1.0$ . The  
549 impact of the input parameters on the performance parameters or the sensitivity of the performance parameters to the  
550 input parameters can be quantitatively described by the absolute value of the SRC coefficient. Furthermore, as shown  
551 in Figs. 21 to 23, the sum of the SRC coefficient can reflect the total contributions of the geometric or injection  
552 parameters to a single performance parameter.

553 As illustrated in Fig. 21, at low load, for  $\text{NO}_x$  and soot emissions, the effects of the injection parameters are  
554 more significant compared to the geometric parameters. On the contrary, for heat transfer losses (HTL), the geometric  
555 parameters exert more obvious influences. As for the combustion losses (CL), the effects of the geometric parameters  
556 are equivalent to those of the injection parameters. At mid load, it is seen from Fig. 22 the sensitivity of the soot  
557 emissions and HTL to the input parameters increases, especially for the geometric parameters. For the  $\text{NO}_x$  emissions  
558 and CL, the injection parameters still play more important roles in contrast to the geometric parameters. At high load,  
559 it is seen from Fig. 23 the sensitivity of the performance parameters to the injection parameters increase globally. The  
560 total SRC coefficients of the geometric parameters for the performance parameters are all lower than those of the

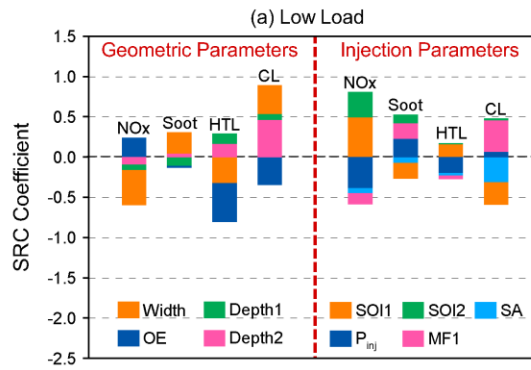
561 injection parameters, except for HTL. This indicates that the fuel injection event becomes more crucial for managing  
562 the engine performance as load increases. Over the whole load range, among the injection parameters, the fuel  
563 injection timings and injection pressure contribute more significant influence to the performance parameters.

564 Overall, from the comparison results of Figs. 21 to 23, the sensitivity of the performance parameters at different  
565 loads can be summarized. For HTL, the geometric parameters contribute more significant effects than the injection  
566 parameters for all loads, although the sensitivity to the injection parameters is increased with at higher load. For CL,  
567 the effects of the geometric parameters are equivalent to those of the injection parameters at low load. With load  
568 increasing, the sensitivity of CL to the geometric parameters decreases, whereas the injection parameters still  
569 contribute obvious influences to the CL at mid and high loads. In terms of the emissions, the NO<sub>x</sub> emissions are more  
570 sensitive to the injection parameters than the geometric parameters over the whole load range. As for the soot  
571 emissions, the influences of both the injection and geometric parameters become more significant as load increases.  
572 Thus, it can be summarized that for HTL, CL, and soot emissions, the sensitivity to the injection parameters is lower  
573 at low load and is higher at mid and high loads. For the NO<sub>x</sub> emissions, the sensitivity to the injection parameters is  
574 lower at low and mid loads. By contrast, at high load, the sensitivity of the NO<sub>x</sub> emissions to the injection parameters  
575 is relatively higher. Overall, it can be concluded that the fuel injection event becomes more important for managing  
576 the engine performance and emissions as load increases

577 Moreover, the key individual input parameters with crucial influences on the performance parameter can be  
578 further summarized as well. Among the geometric parameters, the most influential parameters are Width and Open  
579 Extent (OE), which is also indicated in Ref. [44]. In particular, the two parameters exert obvious and consistent  
580 impacts on heat transfer losses over the whole load range. It is indicated from Figs. 21 to 23 that the heat transfer  
581 losses can be reduced with a wider and more open piston bowl. As for the injection parameters, the fuel injection  
582 timings (*i.e.*, SOI1 and SOI2) and injection pressure (*i.e.*,  $p_{inj}$ ) contribute more influences on the engine performance

583 in contrast to other parameters when load increases.

584

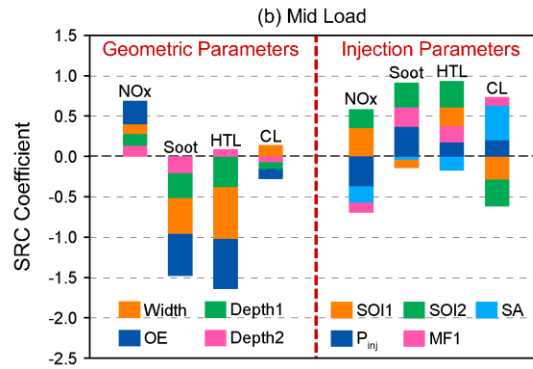


585

586

Fig. 21. SRC coefficient of each input parameter for each performance parameter at low load.

587

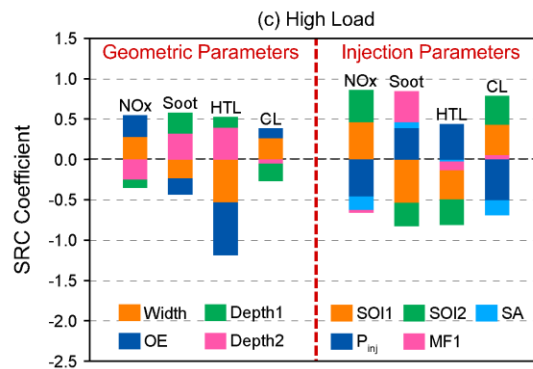


588

589

Fig. 22. SRC coefficient of each input parameter for each performance parameter at mid load.

590



591

592

Fig. 23. SRC coefficient of each input parameter for each performance parameter at high load.

593

## 594 4. Conclusions

595

Based on the DMDF combustion mode, the combined optimization of the piston bowl geometry and the fuel

596 injection strategy was performed over a wide load range using an improved genetic algorithm coupled with the CFD  
597 simulation in this work. The optimal piston bowl shape coupled with the desired injection strategy at different loads  
598 was summarized, and the improvements of engine performance were analyzed compared with the previous results  
599 about the DMDF studies. Furthermore, a correlation analysis was conducted to investigate the sensitivity of engine  
600 performance to the geometric parameters and the injection parameters. The major conclusions can be summarized as  
601 follows.

- 602 1. By optimizing the piston bowl geometry coupled with the injection strategy, the behavior of the DMDF  
603 combustion mode is further enhanced at various loads. Over the test load range, the thermal efficiency is  
604 increased up to 1.4%, 4.4%, and 1.4% for the low, mid, and high loads, respectively. An indicated thermal  
605 efficiency up to 51.8% can be realized at mid load with the combined optimization. Meanwhile, for all the optimal  
606 cases, the NO<sub>x</sub> and soot emissions can meet the Euro VI limits.
- 607 2. The optimal piston bowl shape integrated with the corresponding injection strategy is summarized at each load,  
608 providing guidelines for the piston structure design. At low load, both of the re-entrant and open type piston bowl  
609 can be equipped. At mid load, the shallow open piston bowl and the deep re-entrant piston bowl can be utilized.  
610 At high load, the open type piston bowl is preferred. The combustion occurrence location is determined by the  
611 combined effect of the piston bowl geometry and the injection strategy. Overall, the re-entrant type or deep piston  
612 bowls are good at organizing strong in-cylinder flow, which is beneficial for the fuel/air mixing.
- 613 3. The fuel injection event becomes more important for managing the engine performance and emissions as load  
614 increases. Among the injection parameters, fuel injection timings (*i.e.*, SOI1 and SOI2) and injection pressure  
615 (*i.e.*,  $p_{inj}$ ) contribute more influences on the engine performance and emissions.
- 616 4. The piston bowl geometric parameters contribute more significant effects on the heat transfer losses than the  
617 injection parameters for all loads, although the sensitivity to the injection parameters is increased with the higher

618 load. Among the geometric parameters, the most influential parameters are Width and Open Extent (OE). The  
619 heat transfer losses can be reduced with a wider and more open piston bowl.

620 The future research work will be focused on applying the numerical optimization results in practical engine  
621 experiments. The optimized piston bowl shapes at different loads are will also be integrated into one general shape  
622 for simultaneously considering engine performance and emissions at various operating conditions.

623

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1 Computational optimization of the piston bowl geometry for the different  
2 combustion regimes of the dual-mode dual-fuel (DMDF) concept through an  
3 improved genetic algorithm  
4

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23 Computational optimization of the piston bowl geometry for the different  
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31  
32 **Abstract**

33 Focusing on the dual-mode dual-fuel (DMDF) combustion concept, a combined optimization of the piston bowl  
34 geometry with the fuel injection strategy was conducted at various loads. An improved genetic algorithm was  
35 introduced in this study, which is superior in searching for the global optimal solutions. The optimal piston bowl  
36 shape coupled with the corresponding injection strategy was summarized at the various loads. The results show that  
37 the piston bowl geometry optimization can further improve the thermal efficiency with 1.4%, 4.4%, and 1.4%  
38 percentage points for the low, mid, and high loads, respectively. An indicated thermal efficiency up to 51.8% can be  
39 realized at mid load. Meanwhile, for all the optimal cases, NO<sub>x</sub> and soot emissions can meet the Euro VI limits.

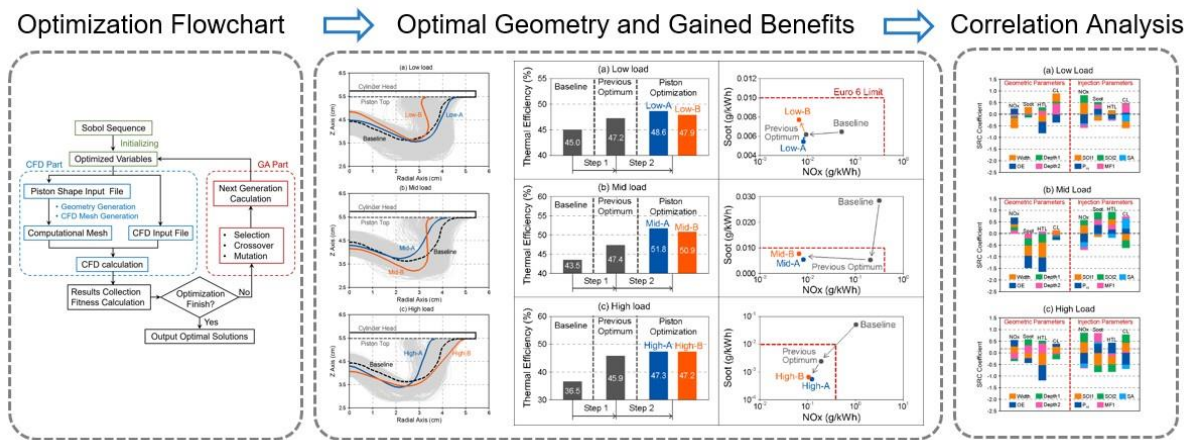
40 At low and mid loads, both the open and re-entrant type piston bowl can be equipped, while the high load only  
41 prefers the open type piston bowl for the DMDF mode. The re-entrant type or deep piston bowls are superior in  
42 organizing strong in-cylinder flow, which is beneficial for the fuel/air mixing. The open type or shallow piston bowls  
43 are helpful for reducing the heat transfer losses owing to the less heat transfer surface area. Furthermore, a correlation  
44 analysis was conducted to investigate the sensitivity of engine performance to the piston geometric parameters and

45 injection parameters. It is concluded that the fuel injection event becomes more important for managing the engine  
 46 performance as load increases. Among the injection parameters, the influence of the fuel injection timings and  
 47 injection pressure on engine performance is more obvious. The piston geometric parameters play more significant  
 48 roles in the heat transfer losses than the injection parameters for all loads. Among the geometric parameters, the most  
 49 influential parameters are the width and open extent of the piston bowl. The heat transfer loss energy fraction can be  
 50 well decreased with a wider and more open piston bowl.

51 **Keywords:** Piston bowl geometry optimization; Dual-mode dual-fuel (DMDF); Genetic algorithm; Fuel efficiency;  
 52 Correlation analysis

53

54 **Graphical abstract**



55

56

## Nomenclature

1D	one-dimensional	IVC	intake valve closing
3D	three-dimension	LHV	lower heating value
ATDC	after top dead center	LTC	low-temperature combustion
CA50	50% burn point	MF1	mass fraction of the first injection
CDC	conventional diesel combustion	NSGA	non-dominated sorting genetic algorithm
CFD	computational fluid dynamics	NO <sub>x</sub>	nitrogen oxides
CL	combustion losses	OE	Open Extent
CO	carbon monoxide	$p_{inj}$	injection pressure
DI	direct injection	$p_{ivc}$	inital pressure at IVC timing
D MDF	dual-mode dual-fuel	$p_{max}$	maximum in-cylinder pressure
DOE	design of experiment	PPC	partially premixed combustion
DPF	diesel particulate filter	PPRR	peak pressure rise rate
EGR	exhaust gas recirculation	PR	premix ratio
EISFC	equivalent indicated specific fuel consumption	RCCI	reactivity controlled compression ignition
EPA	Environmental Protection Agency	RI	ringing intensity
GA	genetic algorithm	SA	spray angle
GCR	geometric compression ratio	SCR	selective catalytic reduction
HRR	heat release rate	SOI	start of injection
HC	hydrocarbon	SOI1	start of injection timing for first pulse
HCCI	homogeneous charge compression ignition	SOI2	start of injection timing for second pulse
HTL	heat transfer losses	SRC	Spearman Rank Correlation
HTR	heat transfer rate	TDC	top dead center
ICE	internal combustion engine	$T_{ivc}$	initial temperature at IVC timing
IMEP	indicated mean effective pressure	VVT	variable valve timing
ISFC	indicated specific fuel consumption		

57

58

## 59 1. Introduction

60 The increasingly stringent emission regulations and urgent energy shortage are bringing huge challenges for the  
61 internal combustion engine (ICE) research community. Improving fuel economy and eliminating engine-out  
62 emissions are still the major objectives and main investigation fields for ICE researchers. Currently, the selective  
63 catalyst reduction (SCR) and diesel particulate filter (DPF) systems have been widely adopted by engine  
64 manufacturers as the aftertreatment devices for decreasing nitrogen oxides ( $\text{NO}_x$ ) and soot emissions, respectively.  
65 Although their effectiveness has been demonstrated, the engine layout complexity and cost are increased as well [1].  
66 Alternatively, the low-temperature combustion (LTC) strategy [2] was proposed, which yields great potential of  
67 reducing  $\text{NO}_x$  and soot emissions while maintaining pleasant fuel economy owing to the characteristics of  
68 homogeneous-mixing and low-temperature combustion process.

69 Among the LTC modes, reactivity controlled compression ignition (RCCI) [3] concept attracts more scientific  
70 interest due to the flexible control over the combustion process with the dual-fuel system. In RCCI mode, the fuel  
71 concentration and reactivity stratification can be accomplished relying on delivering the low-reactivity fuel by port  
72 fuel injection (PFI) and the high-reactivity fuel by in-cylinder direct injection (DI), respectively. By adjusting the  
73 low-reactivity fuel percentage and the direct injection event, the fuel distribution and reactivity can be tuned, and a  
74 flexible operation in a wide operating range can be realized [4]. In spite of this, the RCCI strategy is still facing the  
75 problems of low combustion efficiency at low load [5, 6] and serious engine noise at high load [7]. Thus, the  
76 improvement of the RCCI strategy over a wide operating range is still needed.

77 Up to now, many investigations focus on the extension of the RCCI operation range. Lim et al. [8] found that  
78 extremely low  $\text{NO}_x$  and soot emissions, as well as the indicated thermal efficiency of 48.7% can be reached for a  
79 gasoline/diesel RCCI engine at high load up to 21 bar of the indicated mean effective pressure (IMEP). Wang et al.  
80 [9] demonstrated the effectiveness of exhaust gas recirculation (EGR) rate for preventing excessively high peak



81 pressure rise rate (PPRR) and extending the RCCI mode to higher loads. Meanwhile, it was found that the  
 82 employment of gasoline/diesel dual-fuel RCCI mode at mid and high loads can maintain ultra-low NO<sub>x</sub> and soot  
 83 emissions, while the diesel LTC strategy with single fuel injection is more attractive for low load conditions.

84 Molina et al. [10] extended the RCCI operating range by employing a multiple direct-injection strategy  
 85 combined with the Miller cycle. At low load, the double injection strategy was used for managing the combustion  
 86 phasing and emissions. At high load, the injection shifts into a single injection for triggering the ignition and  
 87 maintaining mild combustion. Xu et al. [11, 12] optimized the key parameters of an RCCI engine couple with the the  
 88 variable valve timing (VVT) and variable compression ratio (VCR) strategies at various load conditions. The results  
 89 indicated that the Euro VI limit can be well maintained over the whole load range, whereas the trade-off of the NO<sub>x</sub>  
 90 and soot emissions at high load is difficult to solve. Mikulski et al. [13] found that early intake valve closing is  
 91 beneficial for the RCCI operation at high load, whereas retarding the intake valve opening timing can reduce  
 92 combustion losses.

93 Benajes et al. [14] indicated that 80% of the nominal operating range for conventional diesel engines can be  
 94 covered by the RCCI operation by employing appropriate fuel ratio, EGR rate, and intake temperature, while the  
 95 PPRR limit will not be surpassed. Based on that study, a dual-mode dual-fuel (DMDF) concept was proposed by  
 96 Benajes et al. [15]. In the DMDF concept, the combustion mode was shifted regarding the engine load. At low load,  
 97 the highly-premixed RCCI operation was employed for enhancing the engine efficiency and obtaining low levels of  
 98 emissions. At high load, the combustion mode was switched to diffusive combustion for slowing down the  
 99 combustion rate and meeting the engine mechanical restriction. Recently, a series of efforts were made for the  
 100 development of the DMDF concept, as summarized in Table 1.

101  
 102 Table. 1. A Summary of the main papers published on DMDF combustion mode

Reference	Contents of the research	Main Conclusions
Benajes et al.	The DMDF concept was proposed featuring	• The DMDF concept can fulfill the EURO

[15] (2017)	<p>that the combustion strategy changes as engine load increases.</p> <ul style="list-style-type: none"> <li>• At low loads with the indicated mean effective pressure (IMEP) lower than 8 bar, a fully premixed RCCI strategy is employed;</li> <li>• When engine load rises up to 15 bar, the combustion strategy is switched to highly premixed RCCI mode;</li> <li>• At full load operation, the diffusive dual-fuel combustion is employed.</li> </ul>	<p>VI NO<sub>x</sub> limit up to 14 bar IMEP;</p> <ul style="list-style-type: none"> <li>• Above 5 bar IMEP, the smoke emissions exceed the EURO VI standards for diesel engines, but the majority of the engine map can fulfill the smoke levels below 1 FSN.</li> </ul>
Benajes et al. [16] (2018)	<p>Comparison of the performance and emissions of two dual-mode combustion concepts over different driving cycles using different fuel combinations.</p>	<p>The dual-mode concept has a potential to be implemented in flexible-fuel engines.</p>
García et al. [17] (2019)	<p>Investigation of the effects of the octane number of the low-reactivity fuel at representative operating conditions over the DMDF engine map.</p>	<p>The characteristics of the low-reactivity fuel in the DMDF concept have a major impact on the combustion evolution in a wide range of engine load, speed, low-reactivity fuel fraction, dilution level, and combustion regime.</p>
Macián et al. [18] (2019)	<p>Investigation of the effect of the low-pressure exhaust gas recirculation (LP-EGR) on the gaseous and particle emissions of the DMDF concept fueled with standard gasoline and diesel.</p>	<ul style="list-style-type: none"> <li>• In the fully premixed RCCI mode, the application of the LP-EGR results in high hydrocarbon (HC) and carbon monoxide (CO) emissions;</li> <li>• For the other combustion modes in the DMDF concept, a reduction of the analyzed pollutants is demonstrated with the employment of the LP-EGR compared with the CDC mode.</li> </ul>
Xu et al. [19] (2020)	<p>Optimization of the operating parameters related to the intake condition and fuel injection strategy for strengthening the engine performance of the DMDF concept fueled with gasoline and diesel fuel at various load conditions.</p>	<p>Gross indicated thermal efficiency above 45% is achieved, and the NO<sub>x</sub> and soot emission can be maintained under the Euro VI standard for the whole load range.</p>
García et al. [20] (2020)	<p>Exploring the feasibility of using the fuel blend of oxymethylene ether (OME<sub>x</sub>) and diesel as the high-reactivity fuel instead of pure diesel in the DMDF concept for reducing the</p>	<p>The OME<sub>x</sub>-diesel blends with an OME<sub>x</sub> mass content greater than 70% are able to meet the Euro VI NO<sub>x</sub> standard with ultra-low soot levels (&lt; 0.01 g/kWh) up to 80% engine load.</p>

	lifecycle CO <sub>2</sub> emission.	
García et al. [21] (2020)	Exploration of suitable injector configuration and fuel injection strategy for the DMDF concept with diesel and OME <sub>x</sub> respectively as the high-reactivity fuels.	<ul style="list-style-type: none"> <li>• The long injection durations of OME<sub>x</sub> resulted from its low lower heating value is handled with the employment of the injectors with higher flow rate capacity.</li> <li>• The trade-off relationship between engine-out emissions and the mixing capacity of the injection system is solved, while the engine performance is not significantly affected.</li> </ul>

103

104 Up to date, the DMDF strategy demonstrates superior advantages for balancing load extension and performance  
105 improvement. It has been recognized as a promising dual-fuel combustion concept to satisfy future fuel consumption  
106 and emission regulations [17]. However, for the current DMDF strategy, there still exist some aspects to be further  
107 improved, among which the piston bowl geometry optimization is the most urgent. At present, the piston bowl  
108 geometry for the DMDF strategy is empirically determined. It is well known that the piston bowl geometry can exert  
109 significant influences on engine performance. Moreover, the interactions between the piston bowl structure and the  
110 injection event are crucial for the fuel/air mixture formation and combustion event for the dual-fuel combustion mode.  
111 Thus, the combined optimization of the piston bowl shape with the fuel injection parameters is needed to further  
112 enhance the DMDF combustion characteristics.

113 Up to now, many investigations have been conducted for studying the effects of the piston bowl geometry and  
114 searching for the optimal bowl shape for the engines with advanced combustion concepts. Dempsey et al. [22]  
115 compared the traditional re-entrant type with a modified shallow type piston based on an RCCI engine fueled with  
116 different fuel combinations. It was concluded that the shallow type piston yields better engine efficiency due to lower  
117 heat transfer losses. Similar results were also reported by Park et al. [23] that the shallow type piston bowl can  
118 contribute to a 35% improvement of the gross indicated thermal efficiency. Xu et al. [24] performed an investigation  
119 to study the joint effects of the bowl shape and injection timing based on the partially premixed combustion (PPC)

120 mode and homogeneous charge compression ignition (HCCI) mode. The results indicated that the piston with a  
121 stepped-lip shape is favorable for solving the low-load cold start problem in terms of decreasing the intake  
122 temperature requirement, which is owing to the fact that the fuel-rich regions can be produced in the stepped-lip  
123 piston bowl. Moreover, it was found that the effect of spray/wall interaction is important when the combustion mode  
124 shifts from HCCI to PPC. Nazemian et al. [25] optimized the piston bowl geometry of an RCCI engine by utilizing  
125 CONVERGE software combined with the design of experiment (DOE) method based on the second law of  
126 thermodynamics, and the effects of the main piston bowl shape parameters, including the piston bowl sizes, pip height,  
127 and top land height on exergy destruction were discussed. It was reported that the influence of the bowl diameter and  
128 bowl depth were the most significant of the exhaust heat recovery. The optimization study performed by Lee et al.  
129 [26] indicated that a 9% improvement of fuel consumption with simultaneously reduced NO<sub>x</sub> and soot emissions can  
130 be attained with a shallow type piston bowl and a narrow injection angle for a gasoline/diesel dual-fuel engine.

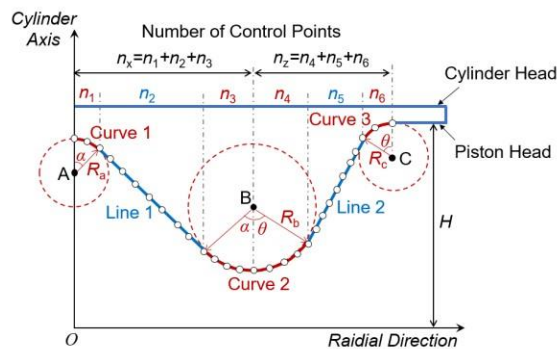
131 From the above literature review, it is confirmed that further optimization of the piston bowl shape used for the  
132 DMDF strategy can lead to potential improvements in fuel efficiency and engine-out emissions. Moreover, up to date,  
133 there have been few studies reporting the piston bowl geometry optimization over a wide load range for the engines  
134 with advanced combustion modes. Thus, in this study, the combined optimization of the piston bowl shape parameters  
135 with the fuel injection strategy was conducted over a wide load range for the DMDF mode based on an improved  
136 genetic algorithm integrated with the computational fluid dynamics (CFD) simulation. Then, the optimal piston bowl  
137 shape coupled with the injection strategy was summarized at different loads. Furthermore, a correlation analysis was  
138 conducted to investigate the sensitivity of engine performance to the geometric parameters and injection parameters,  
139 which can guide the engine structure design.

140

141 2. Computational Method

142 2.1. Generation of the Piston bowl geometry and computational mesh

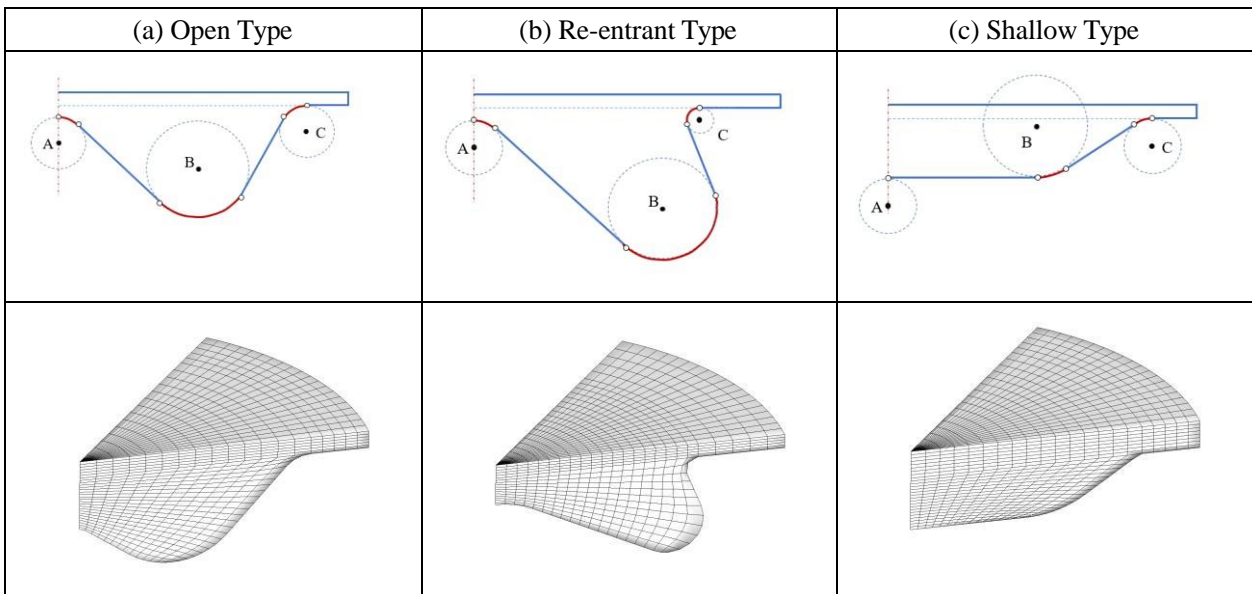
143 In this study, the shape of the piston bowl is generally described using two straight lines (*i.e.*, Line 1 and Line 2) and three circle curves (*i.e.*, Curve 1, Curve 2, and Curve 3) according to the work of Badra et al. [27]. The straight lines and circle curves are represented by the blue and red lines respectively in Fig. 1. It is comprehensible that the shape is determined by the location of circles A, B, and C, as well as their common tangent lines. Thus, the controllable parameters contain the  $X$  and  $Z$  locations of the circle center points A, B, and C, as well as the radius of the three circles, *i.e.*,  $R_a$ ,  $R_b$ , and  $R_c$ . Compared with the traditional method, in which the piston bowl shape is described by the Bezier Curve, the control variables are simplified, and the variable number is cut down to seven with this method. In general, once the coordinates and the radius of the three circles are confirmed, the angles of  $\alpha$  and  $\theta$  (see Fig. 1) can be determined. Thus, the point number and the coordinates of every single point on the piston bowl shape line can be determined, and the piston bowl geometry can be described.



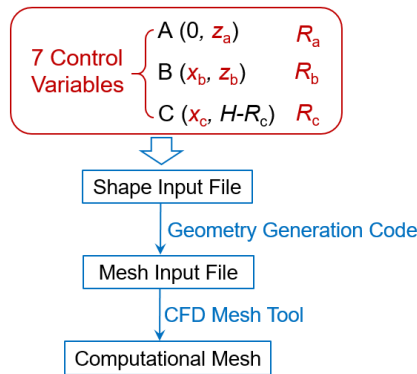
154 Fig. 1. Illustration of automatic generation of the piston bowl geometry.

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157 The common piston bowl geometries widely used in previous studies for advanced combustion modes, including  
158 the Open, Re-entrant, and Shallow piston bowl geometries, can be established using this method, as shown in Fig. 2.  
159 Because the bowl shape is specifically determined by the size and location relationship of the three control circles, it  
160 can be flexibly controlled by the variables shown in Fig. 1 for the optimization of the bowl shape. Fig. 3 illustrates

161 the computational mesh generation process. In this study, the computational mesh is generated using the pre-  
 162 processing tool for mesh establishment in the KIVA code. The input file for the pre-processing program is integrated  
 163 with the geometry generation code according to the shape input file, which includes the information of the three  
 164 control circles (*i.e.*, circles A, B, and C). Among various generated meshes, the computational sector meshes of three  
 165 typical piston bowl geometries with the geometric compression ratio of 14.4 are shown in Fig. 2. It can be seen that  
 166 the computational sector meshes for the Open, Re-entrant, and Shallow piston bowls can be well generated.  
 167



168 Fig. 2. Common piston bowl types and corresponding computational meshes at top dead center.  
 169



170 Fig. 3. Computational mesh generation procedure.  
 171  
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## 173 2.2. CFD Model

174 The CFD calculation of this study was conducted using the open-source KIVA-3V code [28] for simulating the

175 engine working process. Based on the framework of KIVA-3V, several improvements and updates about the sub-  
 176 models have been performed. The turbulence model improved by Wang et al. [29] was used for modeling the in-  
 177 cylinder flow. The improved models were used for modeling the spray impingement [30] and liquid film evolution  
 178 processes [31]. Moreover, the quasi-dimensional model for describing the vaporization processes of fuel droplets [32]  
 179 and liquid films [33] was integrated. Meanwhile, the wall heat transfer model [34], droplet collision model [35], and  
 180 droplet breakup model [36] were also contained in this CFD code. For dealing with the fuel chemistry, the KIVA-3V  
 181 code was coupled with the CHEMKIN solver [37]. Furthermore, the skeletal chemical mechanism constructed by  
 182 Chang et al. [38] was used for predicting the ignition and combustion characteristics of the fuel blends. The diesel  
 183 and gasoline fuel were represented by *n*-heptane and *iso*-octane, respectively. It should be noted that the above models  
 184 have been validated based on numerous experimental data in the previous works, e.g., Refs. [39, 40].

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Table 2. Engine specifications

Bore (mm)	110.0
Stroke (mm)	135.0
Connecting rod length (mm)	212.5
Original compression ratio	14.4:1
Swirl Ratio	2.3
Direct fuel injection system	Common rail
Number of nozzle holes	7
Spray angle (°)	75.0
Nozzle hole diameter (mm)	0.177

187

188 The computational model was validated ahead of the optimization study. Table 2 lists the detailed information  
 189 of the engine tested in this work. The validation was performed at a constant engine speed of 1200 rev/min with  
 190 different IMEP. Table 3 lists the basic conditions and the operating parameters of the validation cases. Table 4 lists  
 191 the the properties of the diesel and gasoline fuels tested in the experiment [15]. Fig. 4 illustrates the computational  
 192 mesh for the original DMDF combustion chamber, and the mesh is generated using the method mentioned above.  
 193 Fig. 5 illustrates the comparison of the simulated and experimental in-cylinder pressure and heat release rate (HRR)

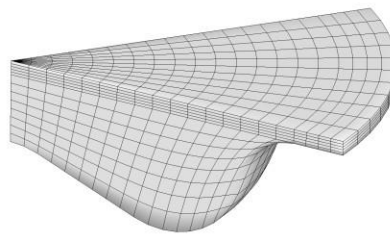
194 traces for five test cases with different IMEP. The comparison results show that the simulated traces can well match  
 195 with the measurements of Benajes et al. [15]. This indicates that the simulation with the generated computational  
 196 mesh can accurately reproduce the combustion process of the DMDF mode at different loads.

197  
 198 Table 3. Basic conditions of the validation cases.

IMEP (bar)	5.9	9.9	11.9	17.3	22.6
$p_{ivc}$ (bar)	1.60	2.29	2.32	3.01	3.09
$T_{ivc}$ (K)	332.6	329.1	347.9	332.2	356.1
EGR rate (%)	19.7	55.5	50.2	45.1	31.0
SOI1 (°CAATDC)	-48.0	-50.0	-45.0	-	-
SOI2 (°CAATDC)	-41.9	-4.4	-5.0	0.0	6.0
Total fuel flow (mg/cycle)	35.5	65.2	81.1	116.9	145.3
Diesel flow (mg/cycle)	31.8	62.3	50.4	52.9	49.3
Gasoline flow (mg/cycle)	3.7	2.9	30.7	64.0	96.0

199  
 200 Table 4. Properties of the diesel and gasoline fuels

	Diesel	Gasoline
Density (kg/m <sup>3</sup> ) @ T=288.15 K	824	720
Viscosity (mm <sup>2</sup> /s) @ T=313.15 K	2.8	-
Research Octane Number (-)	-	95
Motor Octane Number (-)	-	85
Cetane Number (-)	51	-
Lower Heating Value (kJ/kg)	42.92	42.40

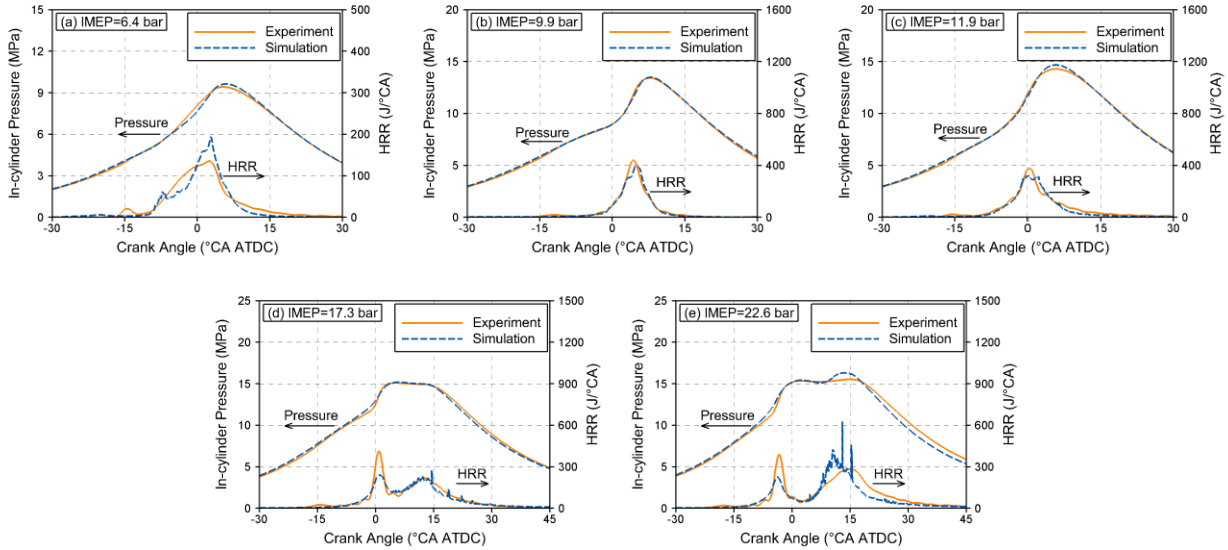


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 203 Fig. 4. Computational mesh for the original DMDF combustion chamber.  
 204

205 Fig. 6 shows comparisons of HC, CO, NO<sub>x</sub> and soot emissions between simulation and experiment. It is found  
 206 that the overall variation trend with varying IMEP can be well captured for the four emissions. However, the  
 207 discrepancies in magnitude still exist between the simulated and experimental emission levels. This is primarily  
 208 owing to the complexity of the in-cylinder flow and fuel/air mixing process, the imperfection of the chemical



209 mechanism [41], and the measurement uncertainties [3]. Since the main task of the simulation tool of this study can  
 210 be qualified by the capability of predicting the emission variation trend as a specific operating parameter changes,  
 211 the computational model and mesh can be employed for the optimization study in the following work.  
 212



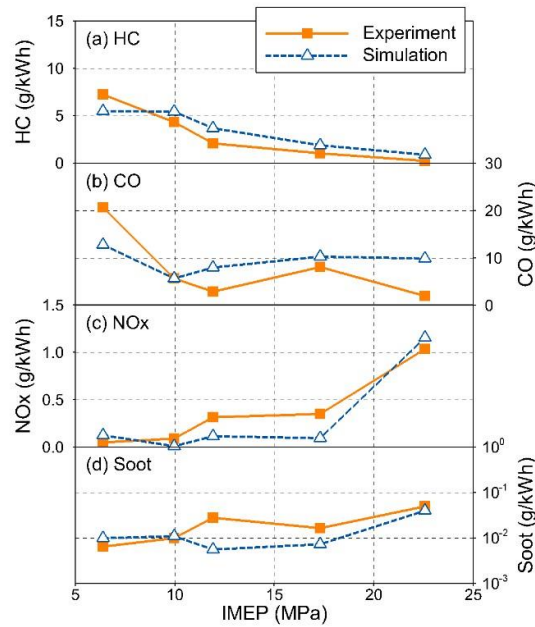
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Fig. 5. Validations of the pressure and HRR at different loads.



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Fig. 6. Validations of the emissions at different loads.

### 2.3. Optimization method

In this study, the optimization of the piston bowl geometry coupled with the injection strategy involves a

222 considerable number of variables. In order to realize the multi-variable multi-objective optimization and  
 223 simultaneously minimize the fuel consumption and engine-out emissions, the non-dominated sorting genetic  
 224 algorithm II (NSGA-II) [42] was utilized. The flowchart of the optimization procedure is illustrated in Fig. 7. The  
 225 global numerical system contains two parts, *i.e.*, the optimization part using GA and the CFD part using KIVA. The  
 226 GA code is coupled with the KIVA code containing the geometry generation code. In the optimization calculation,  
 227 the GA code generates the shape input and CFD input files. The geometry generation code is in charge of exporting  
 228 the mesh input file, which is the input file for the meshing program to create the computational mesh. CFD calculation  
 229 is performed with the CFD input file and the computational mesh. GA code analyzes the CFD calculation results of  
 230 each citizen and generates new data for the next generation calculation.

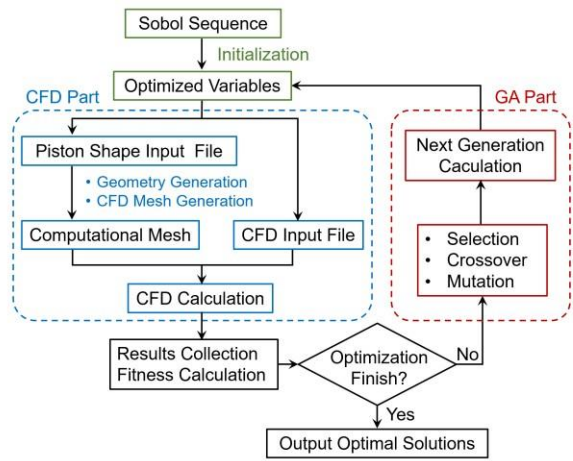
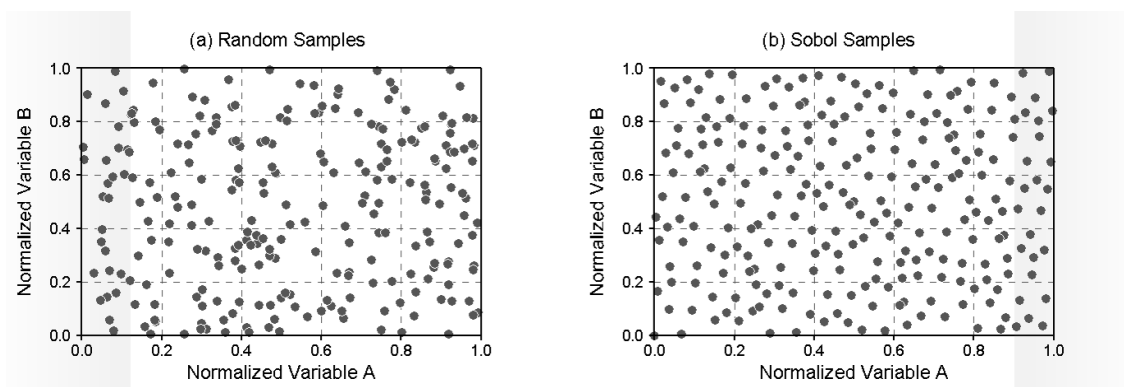


Fig. 7. Illustration of the optimization computation process.

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 234 Considering the increased number of variables, the initial population size needs to be enlarged to keep the  
 235 diversity of the optimal solutions in the GA calculation. In this study, the initialization of the citizens for the first  
 236 generation is improved by introducing the Sobol sequence sampling method [43] instead of the traditional random  
 237 sampling method used in NSGA-II. Fig. 8 shows the distributions of the random samples and Sobol samples with a  
 238 constant sample number of 250 in a two-dimensional variable coordinate. It can be found that the distribution of the  
 239 Sobol samples is more uniform than that of the random samples. This indicates that the Sobol sequence sampling

240 method can provide a better uniformity for the multi-dimensional variables by sufficiently covering the whole  
241 variation ranges of the variables under the conditions with limited population size. Therefore, the introduction of the  
242 Sobol sequence sampling method in this study is aiming at including more possible cases and searching for the global  
243 optimal solutions more effectively, and a relatively small population size can be utilized simultaneously for saving  
244 computational resources.  
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Fig. 8. Comparison of random samples and Sobol samples.

### 249 3. Results and Discussion

#### 250 3.1. Global optimization results

251 In a previous study from the authors [19], based on the diesel/gasoline DMDF combustion concept, the operating  
252 parameters related to the injection strategy and the air intake conditions were optimized to enhance the engine  
253 performance (*i.e.*, Step 1 optimization). A total of seven operating parameters with crucial influences were chosen as  
254 the variables at three different loads in the previous study. Since the injection/wall interaction plays a critical role in  
255 the fuel/air mixture formation, the optimization of the injection parameters cooperated with the piston bowl geometry  
256 was further conducted at different load conditions in this study (*i.e.*, Step 2 optimization). The aim is to search for  
257 the most suitable piston bowl shape for the DMDF combustion mode over a wide load range. A total of 14 parameters  
258 were considered in the present work, including seven geometric parameters and seven engine operating parameters.  
259 The optimization specifications are listed in Table 5.

260  
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Table 5. Optimization specifications

	Parameter	Range
Variables	Premix Ratio	(0.0, 1.0)
	SOI1 (°CA ATDC)	(-80.0, 10.0)
	SOI2 (°CA ATDC)	(SOI1, 10.0)
	MF1	(0.0, 1.0)
	Spray angle (°)	(15, 85)
	Injection Pressure (MPa)	(50, 180)
	Compression Ratio	(12.0, 18.0)
	Normalized $Z_a$	(0.0, 1.0)
	Normalized $Z_b$	(0.0, 1.0)
	Normalized $X_b$	(0.0, 1.0)
	Normalized $X_c$	(0.0, 1.0)
	Normalized $R_a$	(0.0, 1.0)
	Normalized $R_b$	(0.0, 1.0)
Normalized $R_c$	(0.0, 1.0)	
Constraints	EISFC (g/kWh)	<250.0
	$T_{max}$ (K)	>1100.0
	NO <sub>x</sub> (g/kWh)	<0.4
	soot (g/kWh)	<0.01
	PPRR (bar/°CA)	<15.0
	$p_{max}$ (MPa)	<20.0
	RI (MW/m <sup>2</sup> )	<10.0

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Table 6. Initial conditions at IVC timing at each load.

	Low	Mid	High
$p_{ivc}$ (bar)	1.51	1.99	3.30
$T_{ivc}$ (K)	392.2	306.1	315.5
EGR (%)	6.5	6.5	31.0

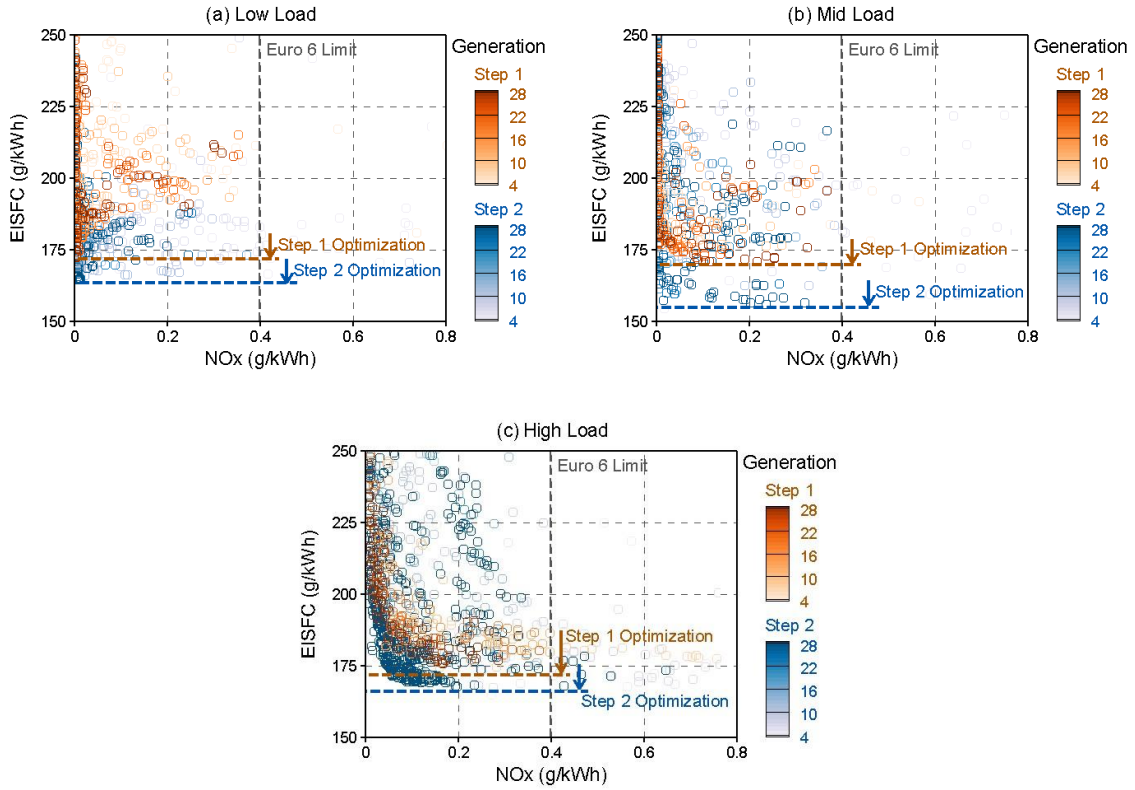
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265 The seven geometric parameters are normalized  $Z_a$ ,  $Z_b$ ,  $X_b$ ,  $X_c$ ,  $R_a$ ,  $R_b$ , and  $R_c$ , which determine the piston bowl  
266 shape, as illustrated in Figs. 1 and 2. The variation ranges of the geometric parameters are all from 0.0 to 1.0. The  
267 operating parameters relating to the direct fuel injection event include the two injection timings (*i.e.*, SOI1 and SOI2),  
268 injection pressure (*i.e.*,  $p_{inj}$ ), mass fraction of the first injection (*i.e.*, MF1), and spray angle (SA). The variation ranges  
269 of the injection parameters can be found in Table 5. The SA is equal to a half of the injection plume included angle.  
270 Moreover, the premix ratio (*i.e.*, PR) of gasoline fuel and geometric compression ratio (*i.e.*, GCR) were also included  
271 in the variables to be optimized. In the engine simulations, the squish height was adjusted to match the desired GCR.

272 During the optimization process, the equivalent indicated specific fuel consumption (EISFC), NO<sub>x</sub>, and soot  
273 emissions are selected as the objectives to urge the populations into the pleasant fuel economy and low-emission  
274 orientation. Meanwhile, several constraints are taken into consideration in order to guarantee the rationality of the  
275 optimal cases. In the optimization calculation, the peak in-cylinder temperature is kept above 1100 K to avoid misfire.  
276 For forbidding rough engine operations, the maximum in-cylinder pressure ( $p_{\max}$ ), ringing intensity (RI), and PPRR  
277 are limited under 19.0 MPa, 10 MW/m<sup>2</sup>, and 15.0 bar/°CA, respectively [15]. The EISFC is restricted under 250  
278 g/kWh to ensure satisfactory fuel economy, while the NO<sub>x</sub> and soot emission limits are set according to the Euro VI  
279 regulations (*i.e.*, 0.4 and 0.01 g/kWh, respectively). Moreover, the operating loads for optimization are located at 5.9,  
280 11.9, and 22.6 bar, which are chosen from the baseline cases validated in Section 2.2. According to our previous  
281 study, the optimized air intake conditions including the initial temperature ( $T_{\text{ivc}}$ ) and pressure ( $p_{\text{ivc}}$ ) at IVC timing, as  
282 well as the EGR rate, are used in this work. Table 6 lists the setup of the initial conditions at the IVC timing for the  
283 optimization calculation at the three loads.

284 The optimization results of the present study are first compared with the previous optimization results to  
285 demonstrate the improvements gained from the piston bowl geometry optimization. Fig. 9 shows the evolution of the  
286 EISFC and NO<sub>x</sub> emissions for all the generated cases in the population at the various loads. The yellow and blue  
287 symbols represent the generated cases in the previous optimization (*i.e.*, Step 1 optimization) and the present  
288 optimization (*i.e.*, Step 2 optimization), respectively. Each case is colored by the generation number. A deeper color  
289 denotes a higher optimization degree. From the comparison of the Step 1 optimization to the Step 2 optimization, it  
290 can be found that EISFC is further decreased after the piston bowl geometry optimization while NO<sub>x</sub> emissions can  
291 still meet the Euro VI limit. The soot emissions of the optimal cases (*i.e.*, the deeper-color symbols) are also below  
292 the Euro VI limit, which is not illustrated in Fig. 9 due to space limitation. This well demonstrates the improvement  
293 of fuel economy without sacrificing the engine-out emissions in the Step 2 optimization. Overall, the above results

294 indicate that the piston bowl geometry optimization further enhances the performance of the DMDF combustion  
295 mode at different loads.  
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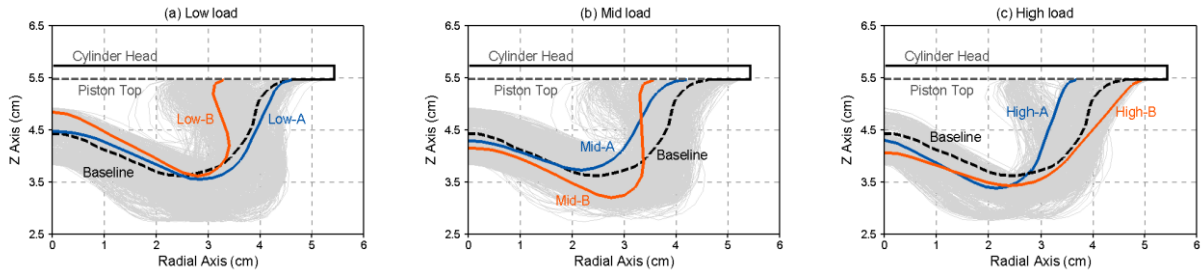
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299 Fig. 9. Evolution of the EISFC and NO<sub>x</sub> emissions during the optimization at different loads.

300

301 Fig. 10 shows the comparison of the piston bowl shapes obtained during the optimization process at different  
302 loads. The dashed black line represents the baseline piston bowl shape for the DMDF mode [15]. The dashed grey  
303 line represents the top dead center position. The solid grey lines denote all the piston bowl profiles generated from  
304 the genetic algorithm. In this section, the cases with competitive fuel efficiency while meeting the Euro VI standards  
305 of the NO<sub>x</sub> and soot emissions are chosen as the optimal cases at each load. Furthermore, in order to provide more  
306 options for the DMDF piston bowl geometry design, among the optimal piston bowls, two typical shapes with  
307 distinguishing geometric characteristics are picked up to represent the optimal piston geometry at each load. The  
308 selected optimal cases are named as Low-A and Low-B for low load, Mid-A and Mid-B for mid load, and High-A  
309 and High-B for high load. As shown in Fig. 10, the optimal shapes are represented by the orange and blue lines.

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Fig. 10 Generated piston bowl shapes and typical optimal piston bowl shapes in the optimization at different loads.

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It is seen from Fig. 10 that the optimal bowl geometries at low and mid loads contain both the open type and re-entrant type bowl, whereas the high load only contains the open type bowl. At low load, the optimal re-entrant type bowl (*i.e.*, case Low-B) features a smaller bowl width, while the optimal open type piston bowl (*i.e.*, case Low-A) features a similar bowl width compared with the baseline piston bowl, as shown in Fig. 10(a). At mid load, the optimal open type piston bowl (*i.e.*, case Mid-A) characterizes a relatively larger bowl width and smaller bowl depth, while the optimal re-entrant type bowl (*i.e.*, case Mid-B) characterizes a relatively smaller bowl width and larger bowl depth, as shown in Fig. 10(b). At high load, the two optimal cases feature a smaller bowl width (*i.e.*, case High-A) and a larger bowl width (*i.e.*, case High-B), respectively. Meanwhile, both of the two optimal cases at high load exhibit larger bowl depth compared with the baseline piston geometry, as shown in Fig. 10(c).

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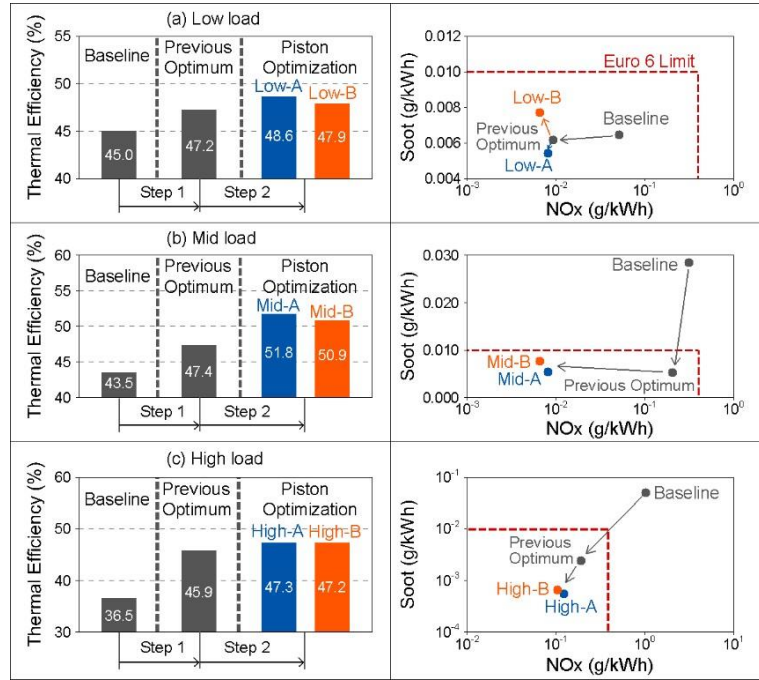
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330

In order to demonstrate the engine improvements using the optimal piston bowl shapes, the optimal cases are compared to the previous optimal cases and the baseline cases in terms of fuel efficiency,  $\text{NO}_x$  and soot emissions, as shown in Fig. 11. The grey bars and symbols represent the baseline cases and the optimal cases from the previous optimization (*i.e.*, Step 1 optimization). The orange and blue bars and symbols represent the optimal cases from the piston bowl geometry optimization (*i.e.*, Step 2 optimization). The left figures illustrate the comparisons of thermal efficiency, and the right figures provide the comparisons for  $\text{NO}_x$  and soot emissions. As depicted in the left sub-figures of Fig. 11, significant improvement can be found for the thermal efficiency with the previous optimization (*i.e.*, Step 1) at the three loads. After optimizing the piston bowl shape combined with the injection parameters (*i.e.*,

331 Step 2), the thermal efficiency is further improved. The thermal efficiency is increased up to 1.4%, 4.4%, and 1.4%  
 332 for the low, mid, and high loads, respectively. It is worth noting that an indicated thermal efficiency up to 51.8% can  
 333 be realized at mid load with the combined optimization. This well demonstrates the benefit gained for fuel economy  
 334 from the piston bowl geometry optimization.

335



336

337 Fig. 11. Comparisons of thermal efficiency, NO<sub>x</sub> emissions, and soot emissions among the baseline cases and the  
 338 optimal cases in Step 1 and Step 2 optimizations.  
 339

340 As for the right sub-figures of Fig. 11, both the NO<sub>x</sub> and soot emissions are continuously decreased after Step 1  
 341 and Step 2 optimizations at high load. At low and mid loads, the improvements of NO<sub>x</sub> and soot emissions for Step  
 342 2 optimization are not as significant as those for Step 1 optimization, but either NO<sub>x</sub> or soot emissions can still be  
 343 further decreased to some extent after Step 2 optimization compared to the cases of Step 1 optimization. For both the  
 344 optimal cases, the NO<sub>x</sub> and soot emissions can meet the Euro VI limits. Thus, it is concluded that the thermal  
 345 efficiency can be significantly improved with the piston bowl geometry optimization without sacrificing NO<sub>x</sub> and  
 346 soot emissions.

347



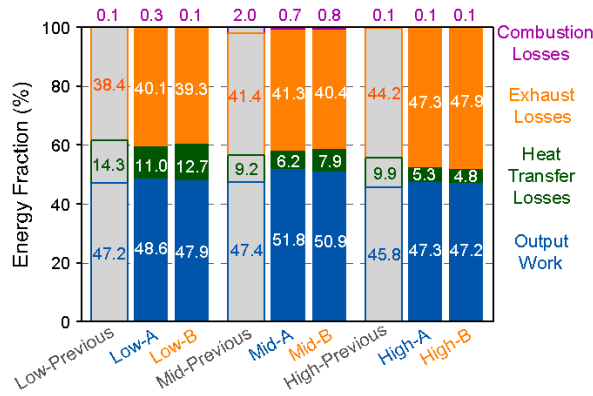
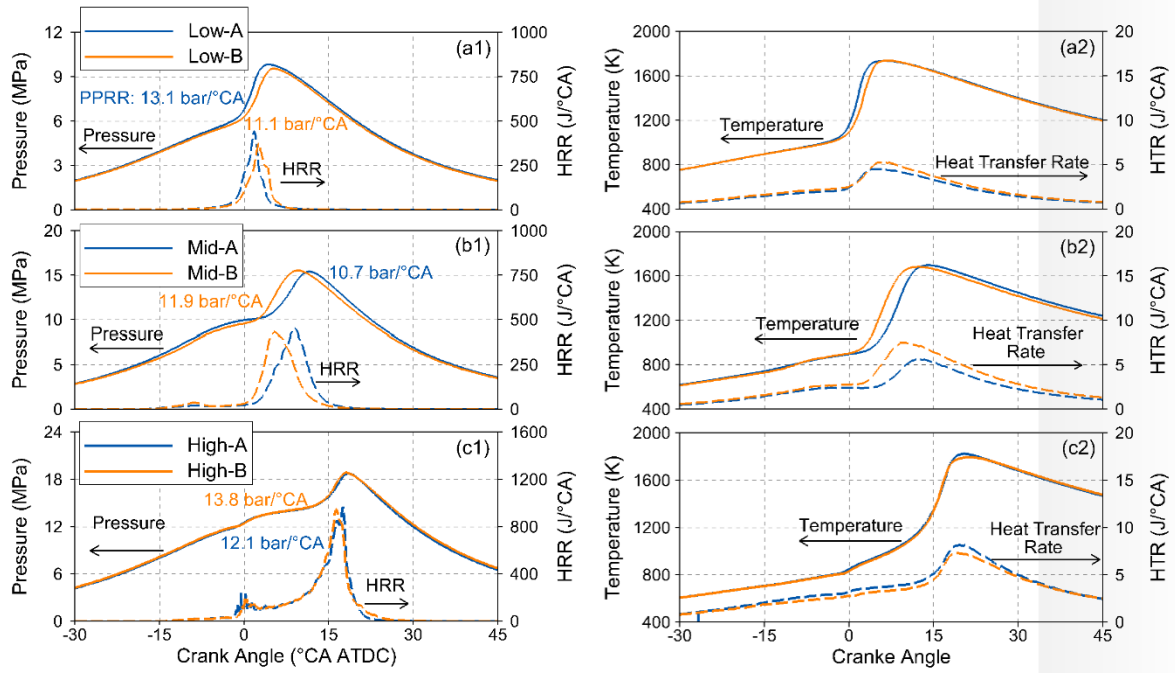


Fig. 12. Illustration of the energy fractions of optimal cases and baseline cases.

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349  
350

351 Furthermore, the energy analysis was conducted for investigating fuel efficiency benefits. As illustrated in Fig.  
352 12, the energy fractions of the optimal cases in Step 2 optimization are compared with those of the previous optimal  
353 cases in Step 1 optimization. The bar colored by grey represents the previous optimal case while the other two  
354 represent the optimal cases from the piston bowl geometry optimization at each load. According to the first law of  
355 thermodynamics, the total input fuel energy is transferred into four parts during the combustion process, including  
356 output work, heat transfer losses, exhaust losses, and incomplete combustion (*i.e.*, combustion losses), as shown in  
357 Fig. 12. It is noted that the energy fraction of output work is directly related to the thermal efficiency depicted in Fig.  
358 11. It can be seen from Fig. 12 that the purple bars are not obviously visible, which is due to the fact that the  
359 combustion losses are relatively low (less than 1%) under the whole load range. This is because that a majority of  
360 HC and CO emissions are reduced by the oxidation reactions in the late combustion stage. Thus, the engine-out  
361 emission levels of HC and CO are low. From the comparison of the optimal cases from the piston bowl geometry  
362 optimization with those from the previous optimization, it can be found that the improvement of the output work (*i.e.*,  
363 thermal efficiency) is mainly resulted from the decrease of the heat transfer losses at low and high loads. At mid load,  
364 the decreases of both the heat transfer losses and combustion losses contribute to the improvement of output work.  
365 This demonstrates the benefits of thermal efficiency gained from the piston bowl geometry optimization.

366



367

368 Fig. 13. Comparison of the in-cylinder pressure, HRR, temperature, and heat transfer rate (HTR) traces between the  
 369 optimal cases.  
 370

371 Furthermore, the combustion process of the optimal cases is analyzed in detail for further explaining the  
 372 improved performance after the piston bowl geometry optimization. Fig. 13 depicts the in-cylinder pressure,  
 373 temperature, HRR, and heat transfer rate (HTR) traces of the optimal cases. Overall, from the comparisons of the  
 374 pressure, temperature, and HRR, it is found that the traces at each load are very similar, especially for the high load  
 375 condition, in spite of slight differences existing in the combustion phasing between the different optimal cases. This  
 376 indicates that the different optimal cases exhibits similar combustion characteristics at each load. In terms of the  
 377 comparison of the three loads, the combustion phasing is found to be retarded with increasing load, which is  
 378 consistent with previous results [11, 19]. This is mainly aiming at controlling ringing intensity and preventing the  
 379 engine knock. It can be seen from the denoted PPRR in Fig. 13 that at mid and high loads, by managing the  
 380 combustion process and combustion phasing, the PPRR can meet the limit of 15 bar/°CA. At low load, although a  
 381 relatively advanced combustion phasing is presented, the PPRR is still under the limit since the released fuel energy  
 382 is much lower than those of mid and high loads.

383 Moreover, in order to understand the heat transfer process, the heat transfer rate (HTR) traces of the optimal  
 384 cases at each load are also illustrated in Fig. 13. By comparing the HTR traces at each load, the differences in the  
 385 heat transfer losses (see Fig. 12) can be explained. It can be found that the global HTR of cases Low-B, Mid-B, and  
 386 High-A is higher than that of cases Low-A, Mid-A, and High-B, respectively. Thus, the heat transfer losses of cases  
 387 Low-B, Mid-B, and High-A are relatively higher. However, the heat transfer process cannot be simply explained by  
 388 the evolution of the global in-cylinder temperature since the piston bowl geometry and the combustion occurrence  
 389 location also play critical roles. Thus, this will be explained in the following section.

### 390 3.2. Typical optimal piston bowl geometry and corresponding injection strategy 391

392 In this section, the optimal piston bowl shape coupled with the corresponding fuel injection strategy is  
 393 summarized at each load. Table 7 lists the operating parameters of each optimal cases. Meanwhile, the fuel injection  
 394 event and the fuel/air mixture formation process are analyzed as well. Fig. 14 shows the liquid fuel distribution after  
 395 injection timing and the equivalence ratio distribution before ignition for cases Low-A and Low-B. As mentioned  
 396 above, the optimal bowl shape for case Low-A is open type, while the optimal bowl shape for case Low-B is re-  
 397 entrant type. Besides, as listed in Table 7, both of the two optimal cases utilize a similar compression ratio with that  
 398 of the original engine setup (*i.e.*, 14.4) [15].

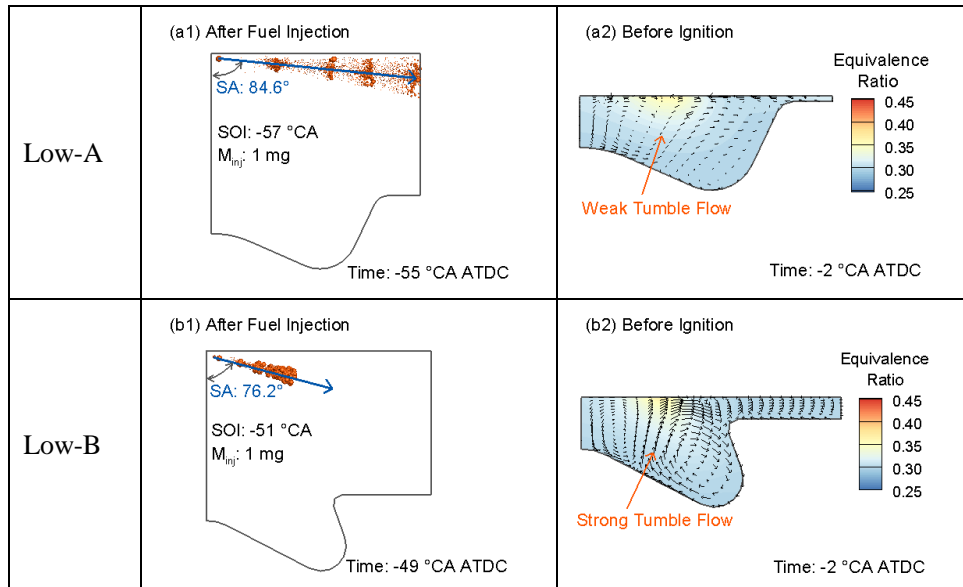
399  
 400 Table 7. Operating parameters of the optimal cases.

	Low-A	Low-B	Mid-A	Mid-B	High-A	High-B
CR	14.6	14.7	16.7	15.8	14.0	13.8
PR	97%	97%	90%	76%	96%	96%
$p_{inj}$ (MPa)	167	101	140	162	176	175
SOI1 (°CA ATDC)	-57	-51	-56	-79	-28	-26
SOI2 (°CA ATDC)	-	-	-51	-60	-15	-18

401  
 402 As for the fuel injection strategy, only the cases with the single injection strategy are retained in the genetic  
 403 algorithm optimization at low load. By comparing Figs. 14(a1) and 14(b1), it is found that case Low-A is coupled

404 with a relatively wider spray angle (SA) of  $84.6^\circ$ . In contrast with case Low-A, case Low-B is coupled with a  
 405 relatively narrower SA of  $76.2^\circ$ , which is similar to that of the original experimental setup (*i.e.*,  $75^\circ$ ) [15]. Figs. 14(a2)  
 406 and 14(b2) illustrate the in-cylinder equivalence ratio distributions before ignition for cases Low-A and Low-B,  
 407 respectively. From the comparison, it can be found that the high fuel concentration locations of the two cases are  
 408 similar, which is owing to the combined effects of the piston bowl geometry and the fuel injection event. As can be  
 409 seen, a stronger tumble flow is organized in the re-entrant piston bowl geometry in contrast to the open type bowl,  
 410 which is also indicated by Miles and Andersson [44], as well as Lee et al. [45]. This results in larger flow velocity  
 411 around the cylinder head and the piston wall near top dead center (TDC) for case Low-B. Thus, although a relatively  
 412 lower injection pressure ( $p_{inj}$ ) and a later SOI timing are employed for case Low-B, the injected fuel can also  
 413 propagate to the similar location as that of case Low-A.

414



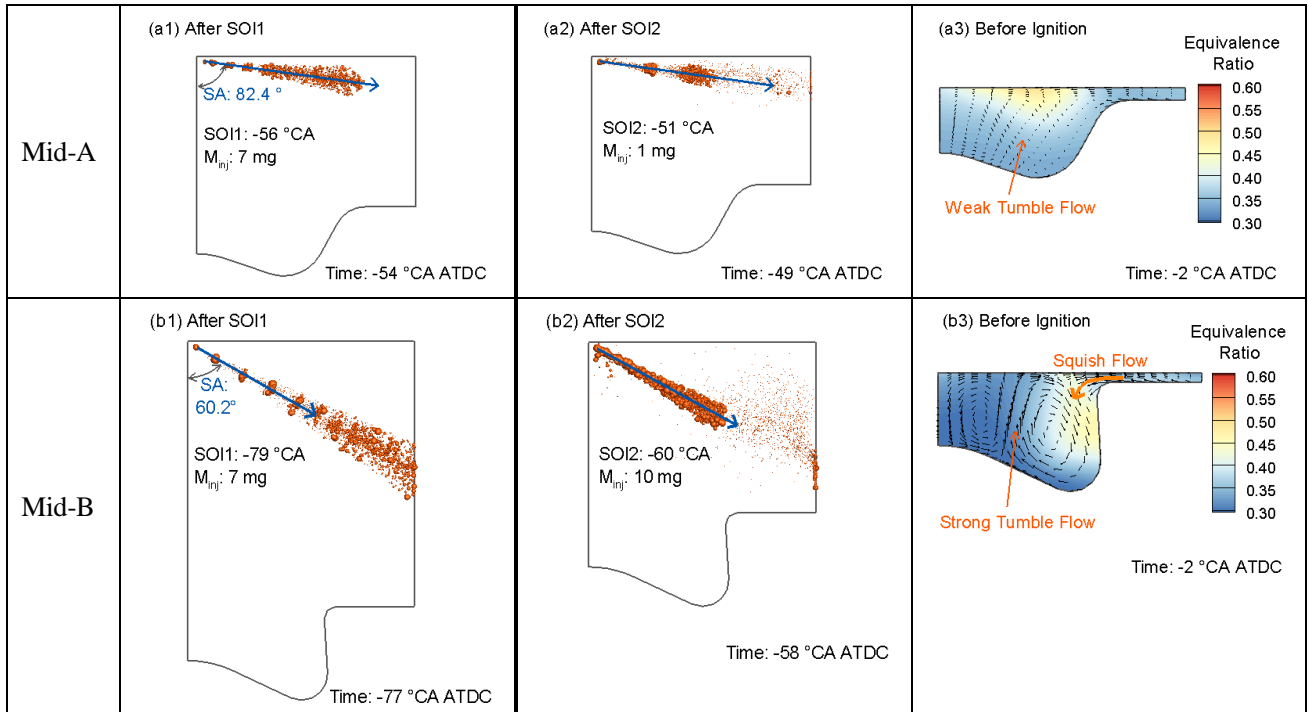
415 Fig. 14. Illustration of the optimal piston bowl shape, fuel injection and the fuel/air mixture formation at low load.

416

417 Fig. 15 depicts the liquid fuel distribution after injection timing and the equivalence ratio distribution before  
 418 ignition for the optimal cases at mid load (*i.e.*, cases Mid-A and Mid-B). The shallow open piston bowl of case Mid-  
 419 A is coupled with a relatively wider SA and lower injection pressure, as well as later fuel injection timings. On the  
 420 contrary, the deep re-entrant piston bowl of case Mid-B is integrated with a relatively narrower SA and higher

421 injection pressure, as well as earlier fuel injection timings. For case Mid-A, due to the lower  $p_{inj}$  and wider SA  
 422 compared to that of case Mid-B, the fuel spray penetration is relatively shorter, and the fuel mainly concentrates near  
 423 the cylinder head, as shown in Fig. 15(a3), which is similar to the situation at low load. For case Mid-B, owing to the  
 424 higher  $p_{inj}$  and earlier fuel injection timings, the fuel penetration spray is much longer, which takes more fuel into the  
 425 squish region. However, the strong squish flow in case Mid-B brings most of the injected fuel back into the bowl  
 426 region, as shown in Fig. 15(b3). Meanwhile, the strong tumble flow resulted from the deep piston bowl geometry is  
 427 helpful for the fuel/air mixing in case Mid-B with the employment of more injected fuel. Furthermore, as listed in  
 428 Table 4, relatively higher CRs are employed in cases Mid-A and Mid-B for strengthening fuel efficiency. Thus, a  
 429 significant improvement in thermal efficiency can be seen in Fig. 11. Meanwhile, with the help of lower initial  
 430 temperature (see Table 3), the combustion phasing can be well controlled and the PPRR limit is maintained at mid  
 431 load.

432



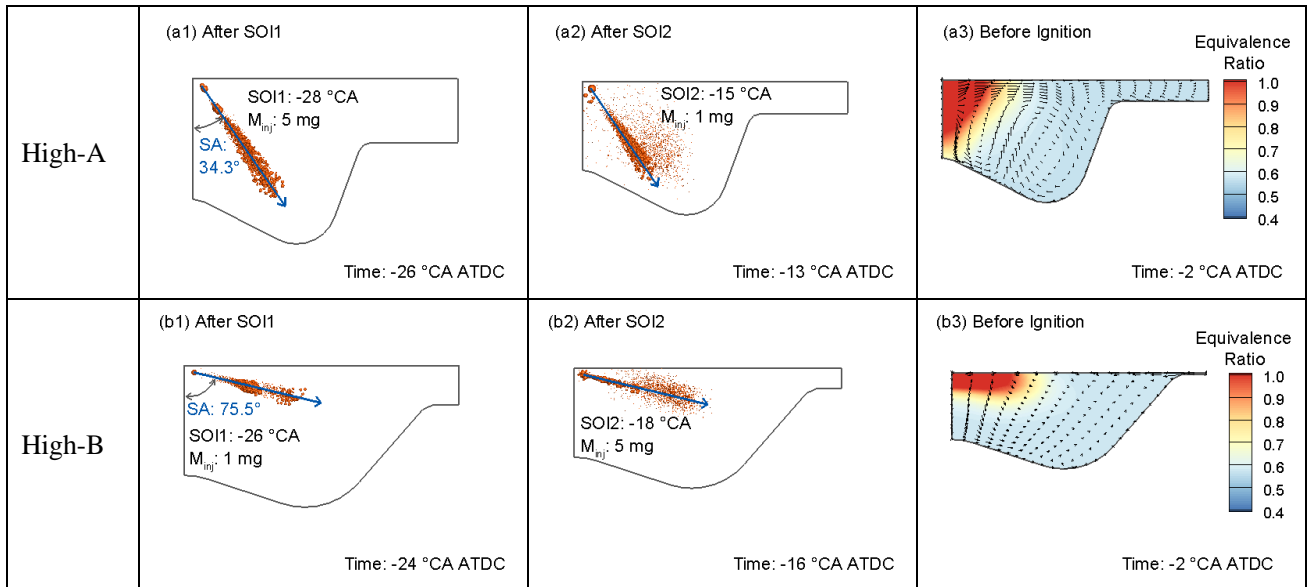
433 Fig. 15. Illustration of the optimal piston bowl shape, fuel injection and the fuel/air mixture formation at mid load.

434

435 As for high load, as shown in Fig. 16, both cases High-A and High-B employ the open type piston bowl. The

436 difference is that case High-A utilizes a deep-narrow bowl geometry, while case High-B employs a shallow-wide  
 437 open bowl geometry. Moreover, case High-A is coupled with a narrower SA, whereas case High-B uses a wider SA.  
 438 In terms of fuel injection timings, both of the SOI1 and SOI2 timings of cases High-A and High-B are retarded  
 439 compared with those of the optimal cases at low and mid loads. This is for avoiding advanced ignition, which can  
 440 lead to high pressure rise rate and consequently engine knock at high load. Meanwhile, the relatively lower  
 441 compression ratio employed by cases High-A and High-B (see Table 4) is also beneficial for controlling the PPRR.  
 442 In such a way, a large fraction of gasoline can be premixed for the DMDF combustion mode at high load without  
 443 exceeding the PPRR limit. Therefore, as shown in Table 4, the premix ratio of cases High-A and High-B can be  
 444 increased to an equivalent level as that of mid and low loads. This is helpful for controlling the NO<sub>x</sub> and soot  
 445 emissions owing to the premixed combustion enhancement.

446

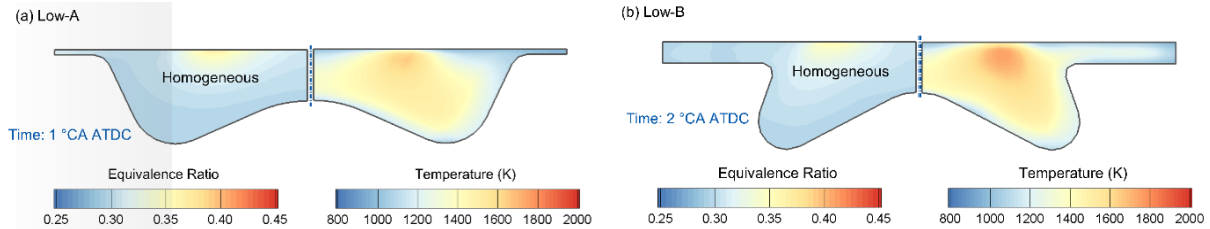


447 Fig. 16. Illustration of the optimal piston bowl shape, fuel injection and the fuel/air mixture formation at high load.

448

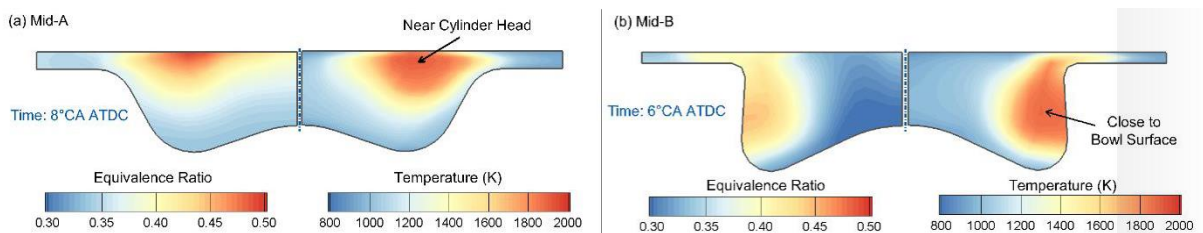
449 The late injection timings combined with the less injected fuel mass result in shorter fuel penetrations for cases  
 450 High-A and High-B. Moreover, although the injection pressure is higher than lower loads (see Table 4), the increasing  
 451 in-cylinder charge density resulted from the higher intake pressure at high load (see Table 3) restricts the propagation  
 452 of the injected diesel fuel. Thus, the injected fuel mainly concentrates around the injection nozzle region, as shown

453 in Figs. 16(a3) and 16(b3). Furthermore, from the comparison of the flow field of cases High-A and High-B, it is  
 454 confirmed again that the deep and narrow bowl geometry can produce strong tumble flow compared with the shallow  
 455 and wide piston geometry.



457  
 458 Fig. 17. In-cylinder equivalence ratio and temperature distributions at CA50 for cases Low-A and Low-B.  
 459

460 In order to further investigate the combustion characteristics of the optimal cases, the in-cylinder temperature  
 461 and equivalence ratio distributions during the combustion process are further analyzed in this section. Figs. 17 to 19  
 462 depicts the in-cylinder temperature and equivalence ratio distributions at the time of 50% burning point (CA50) for  
 463 the optimal cases of low, mid, and high loads, respectively. It can be found that the locations of the high fuel vapor  
 464 concentration and the combustion occurrence are directly related to the fuel distribution pattern before ignition shown  
 465 in the above figures, which is determined by the joint effects of piston bowl geometry and fuel injection strategy. As  
 466 shown in Fig. 17, since the direct-injected fuel mass is lower, and a majority of fuel is premixed in the intake port,  
 467 both cases Low-A and Low-B exhibit a homogeneous equivalence ratio distribution. This leads to the corresponding  
 468 homogeneous combustion characteristics for both the optimal cases, which is helpful for the NO<sub>x</sub> and soot emission  
 469 control. This is consistent with the previous results at low load operation [19].

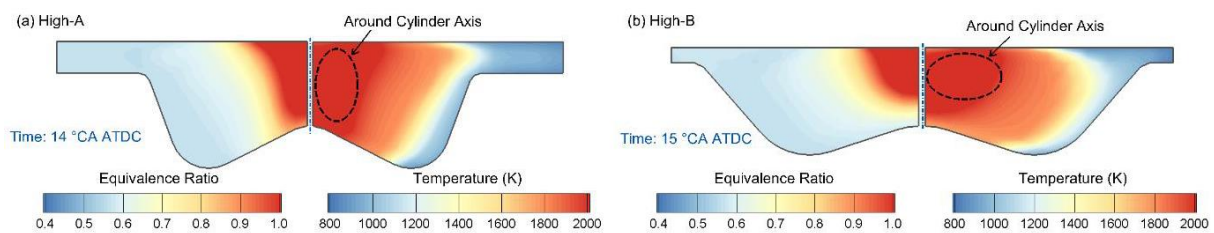


471  
 472 Fig. 18. In-cylinder equivalence ratio and temperature distributions at CA50 for cases Mid-A and Mid-B.  
 473

474 At mid load, with the increase of the injected fuel mass, the local equivalence ratio concentration is increased  
 475 compared with the low load, as seen in Fig. 18. For case Mid-A, consistently with the low-load optimal cases, a high  
 476 premix ratio (see Table 4) is utilized for enhancing the premix combustion, leading to pleasant  $\text{NO}_x$  and soot  
 477 emissions. For case Mid-B, although a higher direct-injected diesel fuel mass (*i.e.*, lower premix ratio) is employed,  
 478 the local equivalence ratio concentration is lower than that of case Mid-A. This is because that the optimized deep  
 479 re-entrant piston bowl geometry of case Mid-B produces a stronger tumble flow within the bowl region, leading to  
 480 more sufficient premixing of the injected fuel with the in-cylinder charge before the combustion occurs. Thus, the  
 481 Euro VI emission limits for the  $\text{NO}_x$  and soot emissions can also be maintained for case Mid-B. Moreover, consistent  
 482 with the vapor distribution of the direct-injected diesel fuel before ignition (see Fig. 15), the combustion occurrence  
 483 location is near the cylinder head and close to the bowl surface for case Mid-A and case Mid-B, respectively.

484 At high load, although the injected mass is not further increased, the local equivalence ratio concentration is  
 485 considerably elevated for the optimal cases, as illustrated in Fig. 19. This is mainly due to the shorter fuel spray  
 486 penetration resulted from the later fuel injection timing and the increased in-cylinder charge density. Correspondingly,  
 487 the combustion occurs near the cylinder axis region, which places the high-temperature region away from the piston  
 488 bowl surface or the cylinder wall during the combustion phasing.

489



490

491

Fig. 19. In-cylinder equivalence ratio and temperature distributions at CA50 for cases High-A and High-B.

492

493 Moreover, the differences existing in the energy fraction of the heat transfer losses (see Fig. 12) between the  
 494 optimal cases at each load can be further explained in this section. At low load, it is easy to find that the re-entrant  
 495 type bowl of case Low-B exhibits a larger surface area compared with the open type bowl. Thus, although there is

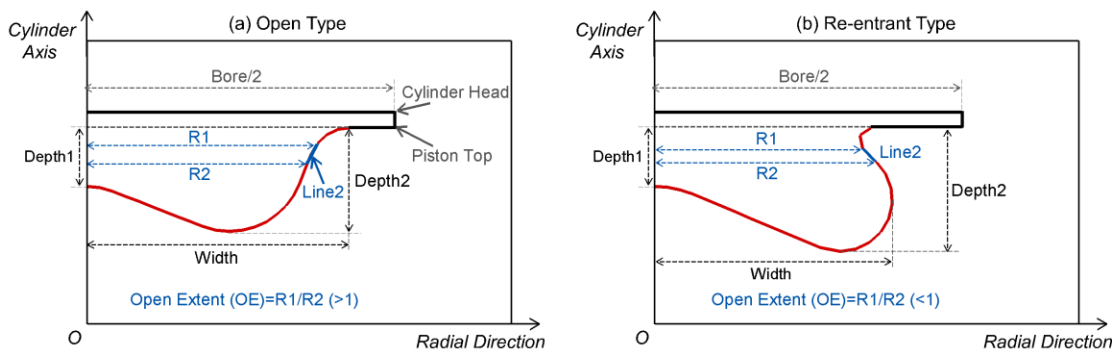


496 no obvious difference in the combustion temperature between cases Low-A and Low-B, the heat transfer energy  
497 fraction of case Low-B is higher than that of case Low-A due to the larger heat transfer area. Similarly, at mid load,  
498 the deep re-entrant piston bowl of case Mid-B yields a larger heat transfer surface. Meanwhile, for case Mid-B, the  
499 high-temperature region is closer to the bowl surface. Therefore, the heat transfer energy fraction is higher for case  
500 Mid-B than case Mid-A. At high load, as mentioned above, the high-temperature regions are away from the bowl  
501 surface for both the two optimal cases. This is beneficial for reducing heat transfer losses. Moreover, although the  
502 two optimal cases at high load employ the open type piston bowl, the heat transfer surface area of case High-B is  
503 smaller due to the opener and wider bowl geometry. Thus, the heat transfer energy fraction of case High-B is slightly  
504 higher than that of case High-A (see Fig. 12).

### 505 506 3.3. Correlation analysis

507 From the above discussion, it can be summarized that the in-cylinder fuel/air mixture formation and combustion  
508 processes are affected by the piston bowl geometry and the fuel injection strategy simultaneously. Thus, the  
509 performance of the DMDF combustion mode directly depends on the combined effects of the geometric parameters  
510 and the fuel injection parameters. For further understanding the influences of these parameters on the DMDF  
511 combustion mode, a correlation analysis was conducted to investigate the sensitivity of the engine performance to  
512 the various parameters at each load in this section. It is noted that 14 parameters were considered as the optimization  
513 variables in this study, which results in the significant complexity of the correlation analysis. Fortunately, a large  
514 number of cases (*i.e.*, citizens) were generated in the GA calculation process. In addition, with the introduction of the  
515 Sobol sequence sampling method for GA in this study, the distribution uniformity for the multi-dimensional variables  
516 of the numerous cases can be ensured, which provides a high-quality database for the correlation analysis in this  
517 section. The aim of the correlation analysis is to investigate the influence weight of each input parameter to the  
518 performance parameter including emissions for the DMDF concept.

519 Before the correlation analysis, the seven geometric parameters (see Fig. 3) were cut down and transferred into  
520 four key parameters for simplifying the analysis complexity. Fig. 20 depicts the definitions of the four new geometric  
521 parameters, including Depth1, Depth2, Width, and Open Extent (OE). The variable of Width is defined as the distance  
522 from the cylinder axis to the right edge of the piston bowl. Moreover, as indicated in Fig. 1, the piston bowl profile  
523 consists of two lines and three circle curves. The type of the piston bowl is directly determined by the orientation of  
524 Line2. Thus, in this section, a new parameter, *i.e.*, Open Extent, is introduced to describe the piston bowl type. The  
525 definition of Open Extent can be found in Fig. 20, which is equal to the ratio of R1 to R2 where R1 and R2 are the  
526 distances from the cylinder axis to the endpoints of Line2. Overall, the four new geometric parameters can well reflect  
527 the piston bowl characteristics.  
528



529  
530 Fig. 20. Illustration of the key parameters for describing the bowl geometry of different types.  
531

532 Subsequently, the correlation analysis was conducted between the input parameters and the performance  
533 parameters. The input parameters contain the four new geometric parameters and five injection parameters, including  
534 the SOI1, SOI2, MF1, SA, and  $p_{inj}$ . The performance parameters contain the energy fractions of heat transfer losses  
535 (HTL) and combustion losses (CL), as well as the  $NO_x$  and soot emissions, which can reflect the combustion and  
536 emission characteristics of the DMDF engine. In this study, the correlation analysis is performed based on the  
537 Spearman Rank Correlation (SRC) coefficient [46]. This method is capable of providing the statistical relevance  
538 between the model input parameters and the target output parameters, and it has been widely used in engineering

539 applications [47-49]. The SRC coefficient is defined as

$$540 \quad \text{SRC} = \frac{\text{COV}(R_x, R_y)}{\sigma_{R_x} \sigma_{R_y}} \quad (1)$$

541 where  $x$  and  $y$  respectively represent the input and target output parameters,  $R_x$  and  $R_y$  respectively denote the rank

542 values of parameters  $x$  and  $y$ ,  $\text{COV}(R_x, R_y)$  is the covariance of  $R_x$  and  $R_y$ , and  $\sigma_{R_x}$  and  $\sigma_{R_y}$  represent the standard  
543 deviations of  $R_x$  and  $R_y$ . In this study, the samples are chosen from the citizens generated in the GA calculation. After

544 excluding the unreasonable cases with deteriorated combustion efficiency or rough engine operations, around 500  
545 effective cases are retained as the samples for the correlation analysis at each load.

546 Figs. 21 to 23 illustrate the SRC coefficient of each input parameter to each performance parameter at low, mid,  
547 and high loads, respectively. In each figure, the left and right parts depict the SRC coefficient of the geometric  
548 parameters and the injection parameters, respectively. The range of the SRC coefficient is from  $-1.0$  to  $1.0$ . The  
549 impact of the input parameters on the performance parameters or the sensitivity of the performance parameters to the  
550 input parameters can be quantitatively described by the absolute value of the SRC coefficient. Furthermore, as shown  
551 in Figs. 21 to 23, the sum of the SRC coefficient can reflect the total contributions of the geometric or injection  
552 parameters to a single performance parameter.

553 As illustrated in Fig. 21, at low load, for  $\text{NO}_x$  and soot emissions, the effects of the injection parameters are  
554 more significant compared to the geometric parameters. On the contrary, for heat transfer losses (HTL), the geometric  
555 parameters exert more obvious influences. As for the combustion losses (CL), the effects of the geometric parameters  
556 are equivalent to those of the injection parameters. At mid load, it is seen from Fig. 22 the sensitivity of the soot  
557 emissions and HTL to the input parameters increases, especially for the geometric parameters. For the  $\text{NO}_x$  emissions  
558 and CL, the injection parameters still play more important roles in contrast to the geometric parameters. At high load,  
559 it is seen from Fig. 23 the sensitivity of the performance parameters to the injection parameters increase globally. The  
560 total SRC coefficients of the geometric parameters for the performance parameters are all lower than those of the

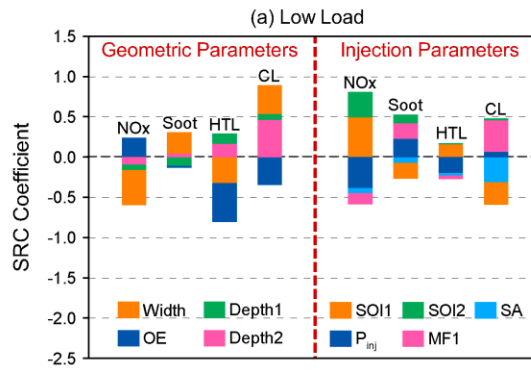
561 injection parameters, except for HTL. This indicates that the fuel injection event becomes more crucial for managing  
562 the engine performance as load increases. Over the whole load range, among the injection parameters, the fuel  
563 injection timings and injection pressure contribute more significant influence to the performance parameters.

564 Overall, from the comparison results of Figs. 21 to 23, the sensitivity of the performance parameters at different  
565 loads can be summarized. For HTL, the geometric parameters contribute more significant effects than the injection  
566 parameters for all loads, although the sensitivity to the injection parameters is increased with at higher load. For CL,  
567 the effects of the geometric parameters are equivalent to those of the injection parameters at low load. With load  
568 increasing, the sensitivity of CL to the geometric parameters decreases, whereas the injection parameters still  
569 contribute obvious influences to the CL at mid and high loads. In terms of the emissions, the NO<sub>x</sub> emissions are more  
570 sensitive to the injection parameters than the geometric parameters over the whole load range. As for the soot  
571 emissions, the influences of both the injection and geometric parameters become more significant as load increases.  
572 Thus, it can be summarized that for HTL, CL, and soot emissions, the sensitivity to the injection parameters is lower  
573 at low load and is higher at mid and high loads. For the NO<sub>x</sub> emissions, the sensitivity to the injection parameters is  
574 lower at low and mid loads. By contrast, at high load, the sensitivity of the NO<sub>x</sub> emissions to the injection parameters  
575 is relatively higher. Overall, it can be concluded that the fuel injection event becomes more important for managing  
576 the engine performance and emissions as load increases

577 Moreover, the key individual input parameters with crucial influences on the performance parameter can be  
578 further summarized as well. Among the geometric parameters, the most influential parameters are Width and Open  
579 Extent (OE), which is also indicated in Ref. [44]. In particular, the two parameters exert obvious and consistent  
580 impacts on heat transfer losses over the whole load range. It is indicated from Figs. 21 to 23 that the heat transfer  
581 losses can be reduced with a wider and more open piston bowl. As for the injection parameters, the fuel injection  
582 timings (*i.e.*, SOI1 and SOI2) and injection pressure (*i.e.*,  $p_{inj}$ ) contribute more influences on the engine performance

583 in contrast to other parameters when load increases.

584

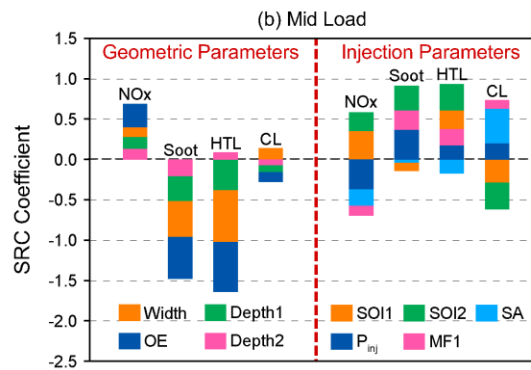


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Fig. 21. SRC coefficient of each input parameter for each performance parameter at low load.

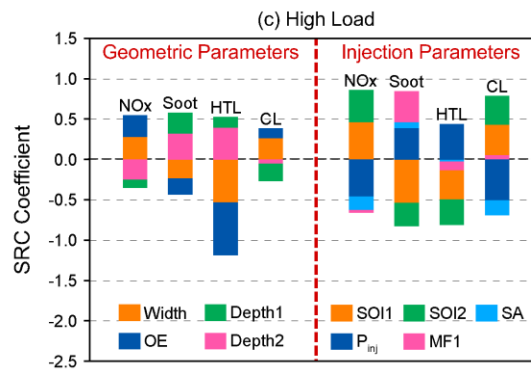


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Fig. 22. SRC coefficient of each input parameter for each performance parameter at mid load.



591

592

593

Fig. 23. SRC coefficient of each input parameter for each performance parameter at high load.

#### 594 4. Conclusions

595 Based on the DMDF combustion mode, the combined optimization of the piston bowl geometry and the fuel

596 injection strategy was performed over a wide load range using an improved genetic algorithm coupled with the CFD  
597 simulation in this work. The optimal piston bowl shape coupled with the desired injection strategy at different loads  
598 was summarized, and the improvements of engine performance were analyzed compared with the previous results  
599 about the DMDF studies. Furthermore, a correlation analysis was conducted to investigate the sensitivity of engine  
600 performance to the geometric parameters and the injection parameters. The major conclusions can be summarized as  
601 follows.

- 602 1. By optimizing the piston bowl geometry coupled with the injection strategy, the behavior of the DMDF  
603 combustion mode is further enhanced at various loads. Over the test load range, the thermal efficiency is  
604 increased up to 1.4%, 4.4%, and 1.4% for the low, mid, and high loads, respectively. An indicated thermal  
605 efficiency up to 51.8% can be realized at mid load with the combined optimization. Meanwhile, for all the optimal  
606 cases, the NO<sub>x</sub> and soot emissions can meet the Euro VI limits.
- 607 2. The optimal piston bowl shape integrated with the corresponding injection strategy is summarized at each load,  
608 providing guidelines for the piston structure design. At low load, both of the re-entrant and open type piston bowl  
609 can be equipped. At mid load, the shallow open piston bowl and the deep re-entrant piston bowl can be utilized.  
610 At high load, the open type piston bowl is preferred. The combustion occurrence location is determined by the  
611 combined effect of the piston bowl geometry and the injection strategy. Overall, the re-entrant type or deep piston  
612 bowls are good at organizing strong in-cylinder flow, which is beneficial for the fuel/air mixing.
- 613 3. The fuel injection event becomes more important for managing the engine performance and emissions as load  
614 increases. Among the injection parameters, fuel injection timings (*i.e.*, SOI1 and SOI2) and injection pressure  
615 (*i.e.*,  $p_{inj}$ ) contribute more influences on the engine performance and emissions.
- 616 4. The piston bowl geometric parameters contribute more significant effects on the heat transfer losses than the  
617 injection parameters for all loads, although the sensitivity to the injection parameters is increased with the higher

618 load. Among the geometric parameters, the most influential parameters are Width and Open Extent (OE). The  
619 heat transfer losses can be reduced with a wider and more open piston bowl.

620 The future research work will be focused on applying the numerical optimization results in practical engine  
621 experiments. The optimized piston bowl shapes at different loads are will also be integrated into one general shape  
622 for simultaneously considering engine performance and emissions at various operating conditions.

623

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