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Additional Information

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# Optimization of the Combustion System of a Medium Duty Direct Injection Diesel Engine by Combining CFD modeling with Experimental Validation

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# 15 Abstract

16 The research in the field of internal combustion engines is currently driven by the needs of decreasing 17 fuel consumption and CO<sub>2</sub> emissions, while fulfilling the increasingly stringent pollutant emissions 18 regulations. In this framework, this research work focuses on describing a methodology for optimizing 19 the combustion system of compression ignition (CI) engines, by combining computational fluid dynamics 20 (CFD) modeling, and the statistical Design of Experiments (DOE) technique known as Response Surface 21 Method (RSM). As a key aspect, in addition to the definition of the optimum set of values for the input 22 parameters, this methodology is extremely useful to gain knowledge on the cause/effect relationships 23 between the input and output parameters under investigation.

24 This methodology is applied in two sequential studies to the optimization of the combustion system of a 25 4-cylinder 4-stroke Medium Duty Direct Injection (DI) CI engine, minimizing the fuel consumption while 26 fulfilling the emission limits in terms of NO<sub>x</sub> and soot. The first study targeted four optimization 27 28 parameters related to the engine hardware including piston bowl geometry, injector nozzle configuration and mean swirl number (MSN) induced by the intake manifold design. After the analysis of the results, 29 the second study extended to six parameters, limiting the optimization of the engine hardware to the bowl 30 geometry, but including the key air management and injection settings. For both studies, the simulation 31 plans were defined following a Central Composite Design (CCD), providing 25 and 77 simulations 32 33 respectively.

The results confirmed the limited benefits, in terms of fuel consumption, around 2%, with constant NO<sub>x</sub> emission achieved when optimizing the engine hardware, while keeping air management and injection settings. Thus, including air management and injection settings in the optimization is mandatory to significantly decrease the fuel consumption, by around 5%, while keeping the emission limits.

Diesel Engine, CFD model, Engine Optimization, Engine Efficiency, Emissions control

37 38

39 Keywords:

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#### 46 **1. Introduction**

47 Research on combustion systems in the frame of Internal Combustion Engines (ICE) for 48 road and rail transport applications is traditionally focused on optimizing the 49 conventional and also the advanced combustion concepts for accomplishing the 50 pollutant emissions standards. Those standards are becoming more difficult to achieve, 51 while increasing the engine thermal efficiency arises an additional objective in order to 52 decrease fuel consumption and then  $CO_2$  emissions. Nowadays, engines provide a good 53 trade-off between pollutant emissions and fuel consumption since they are already 54 optimized, so developing them to reach further improvements becomes a hard task.

55 Experimental optimization is a well-known method due to the simplicity of adjusting air 56 management, injection setting or fuel composition aiming for a better combustion process. Therefore, in the past years most of the research works in the field of diesel 57 58 engine analysis and optimization focused on the injector and combustion chamber 59 design, or even the use of fuels with different properties, have been performed 60 experimentally. Choi et al [1] studied the effect of the bowl geometry and a double row 61 nozzle with 12 holes on the emissions. Atmanli et al [2] used a Response Surface 62 Method for finding the optimum diesel-n-butanol-cotton oil ternary blend ratios also for 63 controlling emissions. This experimental approach has been widely applied also to the 64 analysis and optimization of advanced combustion concepts. Genzale et al [3] measured how the emissions are affected by the chamber geometry operating with the low 65 66 temperature combustion (LTC) concept. Benajes et al [4] investigated the potential of 67 the piston geometry to improve the results provided by the Reactivity Controlled Compression Ignition (RCCI) concept in terms of combustion efficiency and emissions. 68 69 However, the experimental optimization of parameters related to the engine hardware, 70 such as the combustion chamber or the injector geometry is costly in terms of time and 71 resources since it involves piston or injector manufacturing and assembling, together 72 with weeks or even months of intensive testing.

73 Recently, Computational Fluid Dynamics (CFD) is gaining reliability in predicting 74 emissions and combustion characteristics by using properly calibrated and validated 75 models. Then, CFD modeling is a very interesting alternative compared to the 76 experimental approach especially for the optimization of the engine hardware due to its 77 lower requirements in terms of time and resources. Thus, it is worth to develop an 78 optimization methodology based on CFD modeling suitable for not only defining the 79 optimum engine hardware/settings configuration, but also to identify qualitatively and 80 quantitatively the most relevant effects of the variables to be optimized (inputs).

Different studies have been carried out using evolutive methods with really encouraging results related to optimum geometries [5,6] or injection and air management settings [7,8,9,10,12]. These results confirm the suitability of genetic algorithms to find the optimum engine configuration (hardware and/or settings), and how the increasing computational power decreases the time cost of combustion chamber optimization until

86 reasonable values. Without these methods, optimization can be carried out by simply 87 discretizing the variables and performing CFD calculation on every combination of 88 them, nonetheless, this limits the amount of parameters to optimize what leads to simple 89 geometries defined by 1 or 2 parameters. Gafoor and Gupta [11] optimized a bowl 90 geometry defined by a single parameter together with the swirl by simulating 35 91 combinations of them. However, when talking about highly accurate results the amount 92 of iterations required by these evolutive methods to obtain the real optimum (not just a 93 local optimum) are possibly unpredictable and even unacceptable due to the large initial 94 population needed to obtain accurate results [16,17]. Even with the micro-genetic 95 algorithm that requires populations of only 5 individuals, the number of simulations 96 required to reach the optimum is not comparable with RSM methods. Yun and Reitz 97 [14] needed 120 iteration for 4 control parameters and Kim et al. [15] needed 150 98 iterations for 5 parameters compared to 25 and 43 simulations required for a 4 and 5 parameters RSM. As a result, these evolutive methods demand many resources in terms 99 100 of CPU and time, especially when simulating 3D combustion chambers for industrial 101 purposes where that increase in the number of simulations implies months. In addition, 102 as previously commented, the exact number of iterations required for a genetic 103 algorithm optimization is unknown forehand since the termination point is arbitrary in 104 order to assure not obtaining a local optimum from the process, so the number of 105 iterations increases drastically.

106 Traditionally, evolutive methods have been the preferred option to carry out a CFD 107 optimization of ICE, and particularly Compression Ignition (CI) engines. As an 108 alternative, the non-evolutive methods provide a predefined number of iterations that 109 increases with the number of inputs, but for a number of inputs ranging between 4 and 6 110 the total time cost is still lower than that provided by the genetic algorithms, and 111 different studies applying non-evolutive methods have proven their potential. The high 112 reliability and accuracy in the results that the non-evolutive Response Surface Methods 113 (RSM) provide in a CFD optimization is shown in those studies [18,19,21]. Compared 114 to the evolutive methods, the RSM allows obtaining trends and results in any region of 115 the chosen optimization region with the optimized configuration. Those trends can be 116 also obtained using a genetic algorithm after carrying out further post-processing 117 activities, but even in this case the accuracy is lower than that provided by RSM due to 118 the randomness of the training points. Finally, the RSM method has been even applied 119 for other applications as the vehicle on board control of the engine settings to optimize 120 the combustion process [20].

In this framework, the research work reported in the present paper focuses on describing and applying a new methodology for optimizing the combustion system of CI engines based on the RSM approach. The optimization process carried out in this paper is divided in 2 stages, the first one optimizes 4 inputs (2 related to the combustion chamber geometry, swirl number and nozzle included angle (NA)), with results in 25 Paper draft: Optimization of the Combustion System of a Medium Duty Direct Injection Diesel Engine by Combining CFD modeling with Experimental Validation

simulations and the second one considers 6 inputs (2 related to the combustion chamber

127 geometry, 2 related to injection settings and 2 related to air management settings), with

results in 77 simulations. From the considerations in this paper, it can be deducted that

129 results generated following this methodology provided much more information and

130 accuracy than a similar optimization using evolutive methods limited to the same

131 number of simulations.

# 132 **2. Experimental tools**

# 133 Engine characteristics

The experimental data required for the calibration and validation of the CFD model was obtained from a 4-cylinder 4-stroke Medium Duty Direct Injection (DI) CI engine, equipped with a common-rail injection system. Table 1 contains the main engine characteristic, while Table 2 shows the key settings for the reference operating condition.

#### 139

#### Table 1 - Engine main characteristics

Engine data	
Max Torque	550 Nm (1400rpm2200 rpm)
Max Power	128 kW (2200 rpm)
Combustion Chamber	Re-entrant
Bore x stroke [mm]	96 x 102
Bowl width [mm]	62.4
Unitary Displacement [cm <sup>3</sup> ]	738.3
Connecting rod length [mm]	154.5
Geometric compression ratio [-]	15.5
Nozzle hole number	9

140

# Table 2 - Engine operating conditions

<b>Operating conditions</b>			
Speed [rpm]	1200	1600	1800
Fuel mass [Kg/s]	2.71e-4	9.36e-4	1.50e-3
IMEP [bar]	6.5	16.2	24.9
EGR [%]	17.7	13	11.3
Global equivalence ratio [-]	0.6	0.73	0.75
Intake temperature [K]	324.9	313.15	318.9
Boost pressure [bar]	1.15	2.28	3
MSN [-]	2	2	2

#### 142 Test cell characteristics

The engine is assembled into a fully instrumented test cell. An external compressor provides the intake air (oil and water-free) required to simulate boost conditions, while the exhaust backpressure is reproduced and controlled by means of a throttle valve placed in the exhaust line after the exhaust settling chamber. The experimental facility also includes a high pressure EGR system, designed to provide arbitrary levels of cooled EGR.

149 The test cell is equipped with a dedicated air and fuel flow meters, and a set of 150 temperature and pressure sensors to assure the proper operation of the system. Data of 151 O<sub>2</sub>, CO, CO<sub>2</sub>, HC, NO<sub>x</sub>, N<sub>2</sub>O and exhaust gas recirculation (EGR) rate is measured with 152 a state-of-the-art exhaust gas analyzer, while Smoke emissions in Filter Smoke Number (FSN) units are measured by a Smokemeter connected to the exhaust line. Instantaneous 153 154 high frequency signals such as cylinder pressure, pressures at the intake and exhaust 155 ports and energizing current of the injector are sampled with a resolution of 0.2 crank 156 angle degree (degree to top dead center). Cylinder pressure is measured using a state-of-157 the-art piezoelectric sensor. The most important combustion parameters like indicated 158 mean effective pressure (IMEP), maximum cylinder pressure (P<sub>max</sub>), pressure gradient 159 (dP/da), combustion noise, combustion phasing angles and heat release rate (HRR); as 160 well as the initial thermodynamic conditions and wall temperatures required for 161 performing the setup of the CFD model, are calculated from the experimental cylinder 162 pressure signal by means of the in-house combustion analysis software (CALMEC) [22,23]. This 0-Dimensional model simplifies the phenomena occurring inside the 163 164 engine cylinder, so it does not provide any information related to local thermochemical conditions. However, the instantaneous evolution of the energy released by the progress 165 166 of the combustion can be obtained with accuracy by resolving the first law of 167 thermodynamics taking the combustion chamber as the control volume independently 168 from the local conditions where this energy is being released.

Table 3 Accuracy of the instrumentation used in this work

	· · · · · · · · · · · · · · · · · · ·		
Variable measured	Device	Manufacturer/model	Accuracy
In-cylinder pressure	Piezoelectric transducer	Kistler/6125B	±1.25 bar
Intake/exhaust pressure	Piezorresistive transducers	Kistler/4045A10	±0.025 bar
Temp in settling chambers/manifolds	Thermocouple	TC direct/type K	±2.5 °C
Crank angle, engine speed	Encoder	AVL/364	±0.02 deg
NO <sub>x</sub> , CO, HC, O2, CO2	Gas analyzer	HORIBA/Mexa 7100 DEGR	4%
FSN	Smoke meter	AVL/415	±0.025 FSN
Diesel fuel mass flow	Fuel balances	AVL/733S	±0.2 %
Air mass flow	Air flow meter	Elster/RVG G100	±0.1 %

# 170 Injection rate test rig

171 Measurements of injection rate were carried out with an Injection Discharge Rate Curve 172 Indicator (IRDCI) commercial system. The device makes it possible to display and 173 record the data that describe the chronological sequence of an individual fuel injection 174 event. The measuring principle used is the Bosch method [24], which consists of a fuel 175 injector that injects into a fuel-filled measuring tube.

176 The fuel discharge produces a pressure increase inside the tube, which is proportional to

177 the increase in fuel mass. The rate of this pressure increase corresponds to the injection

178 rate. A pressure sensor detects this pressure increase, and an acquisition and display179 system further processes the recorded data for further use.

# 180 **3. Modeling tools**

181 The section below describes the experimental and theoretical tools used to carry out the

research. This brief description focuses only on their most relevant characteristics.

# 183 *CFD model*

184 The StarCD code version 4.18 [25] was used to perform the CFD simulations of the 185 engine combustion system. The axisymmetry of the combustion chamber allow us to 186 create a sector mesh comprising 131360 cells at BDC with periodic boundary 187 conditions after performing a grid convergence study. Each case was calculated as a 188 closed cycle combustion, this is from the closure of the inlet valves to the opening of the 189 exhaust valves (from 246.8 to 463° aTDC with the TDC at 360 deg). The simulations 190 were calculated with 12 cores each with an average time cost of 36 hours per 191 simulation.

192 The combustion model was the ECFM-3z from IFP [26]. Concerning pollutants, NO<sub>x</sub>

were calculated using the extended Zeldovich (thermal) mechanism, where source terms
were obtained from a flamelet library [27]. A two-step Hiroyasu-like model was used
for soot formation and oxidation [28].

196 Concerning the physical sub-models, the diesel spray was simulated with the standard 197 Droplet Discrete Model available in StarCD. Spray atomization and break-up were 198 simulated by means of the Huh-Gosman [29] and Reitz-Diwakar [30] models, 199 respectively. Diesel fuel physical properties were given by the DF1 fuel surrogate [31].

In these simulations, turbulent flow was modelled by means of the RNG k-ε model [32],
with wall-functions based on the model from Angelberger [33] in order to account for
wall heat transfer. An implicit scheme was used for time discretization, while
divergence terms used the second order Monotone Advection and Reconstruction
Scheme (MARS) [25]. Velocity-pressure coupling was solved by means of a Pressure-

Implicit with Splitting of Operators (PISO) algorithm [34]. The reference values usedfor the boundary and initial conditions are shown in Table 4.

207 208

 Table 4 - Cylinder thermodynamic conditions at IVC & combustion chamber mean wall temperatures.

Speed	P <sub>IVC</sub>	m <sub>IVC</sub>	T <sub>IVC</sub>	Y <sub>02</sub>	$\mathbf{Y}_{N2}$	Y <sub>CO2</sub>	Y <sub>H2O</sub>	$\mathbf{T}_{wpis}$	T <sub>wliner</sub>	Twhead
[rpm]	[bar]	[g]	[K]	[%]	[%]	[%]	[%]	[K]	[K]	[K]
1200	1.62	0.86	407	19.88	76	2.85	1.26	425.3	380.1	415.8
1600	3.48	1.77	425	20.06	76.04	2.7	1.2	507.4	406.8	496.8
1800	4.67	2.33	434	20.2	76.07	2.58	1.14	551.9	425.9	546

209 These reference values could not be kept constant for all the simulations due to having 210 EGR and boost pressure as optimization parameters, what has a huge impact on the air 211 composition and thermodynamic conditions and therefore, they were accordingly 212 adjusted in each simulation, assuming constant volumetric efficiency and  $T_{IVC}$ . In a 213 similar way, the calculation of the high pressure loop IMEP in the post-processing is affected by these variations. The IMEP of the closed cycle can only be compared 214 215 against experimental data in relative values, so in order to compare in absolute values, 216 the pressure profiles from bottom dead center (BDC) to intake valve closing (IVC) and 217 from exhaust valve opening (EVO) to BDC were taken directly from experimental 218 results, and adjusted in each simulation according to the corresponding operating 219 conditions.

# 220 Bowl geometry model

221 The generation of the combustion chamber geometry is one of the most time consuming 222 step in an optimization. Bowl shapes are very diverse, which makes it difficult to be 223 adjusted, especially with only a few parameters. However, in order to capture properly 224 the trends of the geometric parameters in the RSM method, the process needs to be consistent, this is, the restrictions of the original bowl have to be maintained. For that 225 226 reason, an in-house code to adjust and resize any bowl contour was developed The basic 227 idea behind the code is to adjust the original geometry with Bezier curves and then 228 readjust the curves iteratively taking into account the restrictions, like for example the 229 maximum width of the bowl is limited by the oil gallery location. Figure 1 shows the 230 reference bowl, adjusted with Bezier curves and compared with variations of the 231 geometry for different values of the geometric parameters.

The Bezier line and control points used to adjust the original bowl can be seen in the figure and it is noticeable how the adjusted profile reproduces the original shape perfectly and the new generated lines, because of the restrictions imposed, keep the main aspects of the bowl.

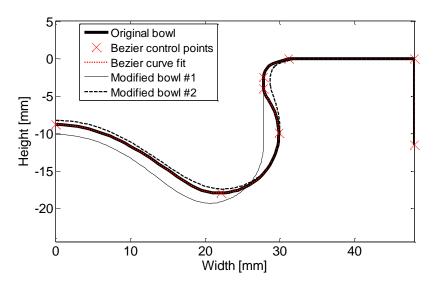




Figure 1 - Bowl geometry profiles: the original bowl with the Bezier polynomial and control points
 and two examples of newly-generated bowl.

#### 239 Injection rate model

240 The injected fuel mass flow rate profile has a critical effect on the combustion process 241 so in order to be consistent with the experimental data, an in-house 0D model code 242 capable of reproducing any injection rate profile was developed. The model needs 243 experimental data because a measured injection rate profile has to be adjusted using 244 Bezier curves and then, the curve generated from adjusting the experimental injection 245 rate profile is modified to fit the required injection pressure and total injected mass. 246 Figure 2a shows the measured injection profile used as reference and the curves obtained from the software and Figure 2b shows the readjusted injection profile and the 247 corresponding experimental data. 248

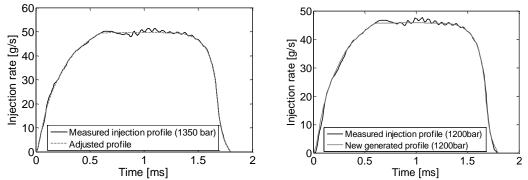




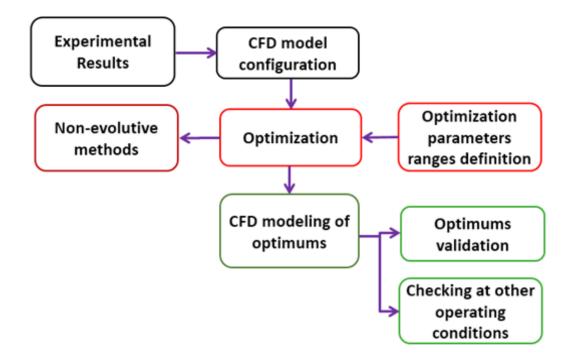
Figure 2 a) Reference injection profile at 1300bar and adjusted curve with Bezier curves. b) New generated profile with the 0D model at 1200bar and the experimental data for 1200bar.

A critical aspect of the injection is the slope of the injection rate when the injector receives the electric signal and when the signal ends. It can be seen in Figure 2 how the injection profile generator keeps the original slopes, what assures the consistency withthe experimental data.

# 256 **4. Methodology**

Accuracy is one of the most difficult aspects when optimizing unknown processes that cannot be tested experimentally. Part of this inaccuracy comes from the CFD model but an important fraction also comes from the optimization methodology. In order to avoid uncertainties due to the combustion process and to be able to validate the methodology, the ranges of the optimization parameters were chosen in order to keep a conventional combustion in all cases so the know-how on this combustion models can be used to validate results and trends.

- 264 The methodology described in this section has 3 steps, while each of them has their own
- tools, which are described in the tools section. Figure 3 shows summarizes the 3 steps ofthe methodology.
- 267

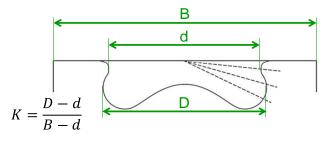


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- 269 270

Figure 3 Flow chart of the methodology steps

The first step is the configuration of the CFD model used for the later optimization. It has to be properly calibrated and validated with experimental data because the main objective of the optimization process is to vary parameters in a given range so not having a well calibrated model could change the trends provided by the engine. It has to be pointed that the calibrated model parameters have been kept constant for the following steps. 277 The second step is dedicated to the optimization of the combustion system. The 278 methodology for this optimization is based on Design of Experiments (DOE) 279 techniques, particularly the Response Surface Method (RSM). This method was 280 selected due to its attractive cost/benefit ratio specially compared to the evolutive 281 optimization methods, which are more costly and less predictable in terms of time. 282 Moreover, due to the randomness of the simulated points, with evolutive methods it is 283 more difficult and less accurate to capture the cause/effect relations between the input 284 and the output parameters.

- The final step focuses on validating the optimums. Once the DOE are performed, a series of convenient optimum are obtained from the response surface and those optimums have to be validated with the CFD model to assure the wanted accuracy of the method. Additional validations at other operating conditions are necessary to check if the new set up has a better performance than the original in well-representative points of the engine map.
- In this study, four parameters for Stage 1 and six parameters for Stage 2 were chosen to be optimized and a Central Composite Design (CCD) defined the DOE test plan with 25 and 77 simulations respectively. Among the output parameters, efficiency, emissions and combustion related parameters were included. The objective of some of these parameters was to confirm the key trends followed by the main outputs.
- 296 Concerning the input factors, the bowl geometry was parameterized by means of two 297 geometrical relations, the ratio between the rip bowl diameter (d) and the cylinder bore 298 (B) and a second parameter (K) defined specifically to control the reentrant shape of the 299 bowl avoiding the artificial generation of extremely deformed bowl shapes. Due to its 300 definition, included in Figure 4 together with the geometry of the central point of the 301 DOE, the higher the K the more reentrant bowl shape. The ranges for the input 302 parameters kept for all DOE are shown in Table 5 and Table 6.



303

**304** Figure 4 – Sketch of the bowl geometry for the central point of the DOE and definition of K factor.

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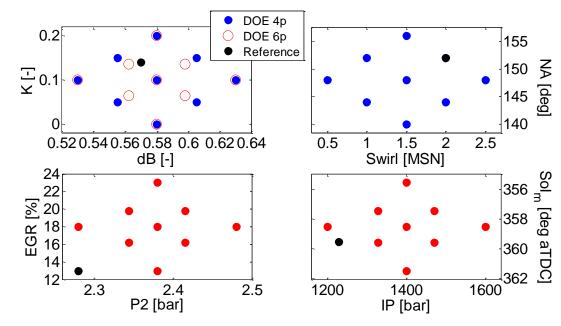
 Table 5 - Ranges for the input factors for the optimization Stage 1 DOE of 4 parameters.

	d/B	K	Swirl	NA
	[-]	[-]	[MSN]	[deg]
Ref	0.57	0.14	2	148
min	0.53	0	0.5	140
max	0.63	0.2	2.5	156

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306	Table 6	- Ranges for t	the input facto	ors for the optim	mization Stage	e 2 DOE of 6 p	parameters.	
		GEOMETRY		AIR M	ANAG.	INJECTION		
		d/B	K	P2	EGR	IP	SoI <sub>m</sub> [deg a	
		[-]	[-]	[bar]	[%]	[bar]	TDC]	
	Ref	0.57	0.14	2.28	13	1230	359.5	
	min	0.53	0	2.28	13	1200	355.5	
	max	0.63	0.2	2.48	23	1600	361.546	

Figure 5 contains the combinations of the 2 parameters related to the bowl geometry
included in the DOE design compared to those of the original engine bowl geometry.
The same comparison is carried out between the other settings modified in the
optimization process.



311312

Figure 5 - Combinations input parameters for Stages 1 and 2.

313 It is important to highlight how despite the well-known trade-off existing between ISFC 314 and BSFC especially when the boost pressure is adjusted, the analysis was carried out 315 considering ISFC and not BSFC since this research focuses on understanding the 316 requirements of the combustion system to optimize the energy conversion from heat to 317 work respecting emission constraints. These processes are intrinsically controlled by the 318 combustion process, while the mechanical losses (including pumping losses) are not 319 accounted for since they depend on external factors not directly controlled by the 320 combustion process such as the lubrication and surface finish (friction losses), the 321 mechanical efficiency of auxiliary systems (auxiliary losses) or the turbocharging 322 system efficiency and its matching (pumping losses). The optimization of the 323 combustion system to obtain the best indicated efficiency carried out in this

324 investigation must be followed by a next step dedicated optimization of the engine 325 subsystems to transfer the ISFC improvements into final BSFC benefits.

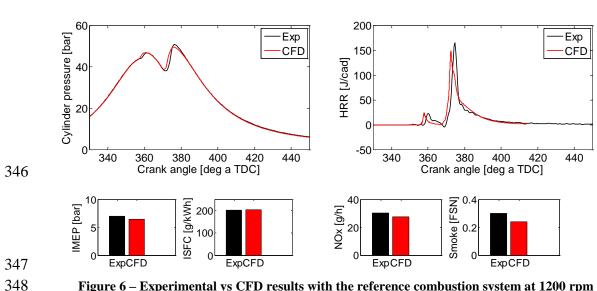
#### 326 5. Results and discussion

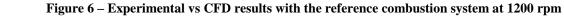
327 The section below describes the CFD model validation and two optimizations 328 performed for the reference engine. The first optimization stage focuses on optimizing 329 four engine parameters (bowl shape, intake manifold design and injection hardware) and 330 the second stage keeps the geometric parameters as optimization inputs and adds four more optimization parameters (injection and air management settings). 331

332 5.1. CFD model calibration and validation

333 The CFD model was thoroughly validated by simulating the three operating conditions 334 under investigation described in Table 2. The results of the CFD model compared 335 against the experimental data in terms of performance and pollutants after calibrating 336 the sub-model constants, especially those related to the soot model, are included in 337 Figure 6, Figure 7 and Figure 8.

338 Those figures show a fair agreement in terms of performance (IMEP), fuel consumption 339 (ISFC) and combustion characteristics (HRR). In addition, the final soot levels were 340 close to experimental data after adjusting the constants of the soot formation model. An over-prediction of NO<sub>x</sub> values is observed for the high load condition, probably related 341 342 with the faster rise on the main HRR compared to experimental data, however, the quality of the CFD model was considered as suitable for carrying out the optimization 343 344 activities.

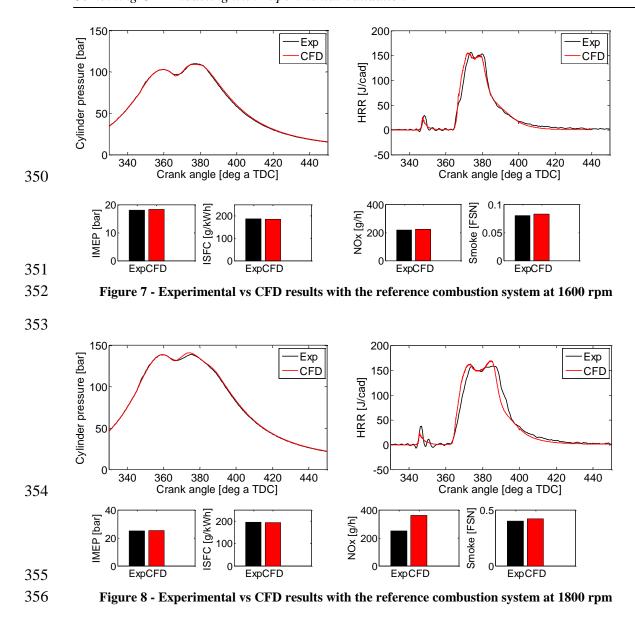


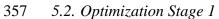


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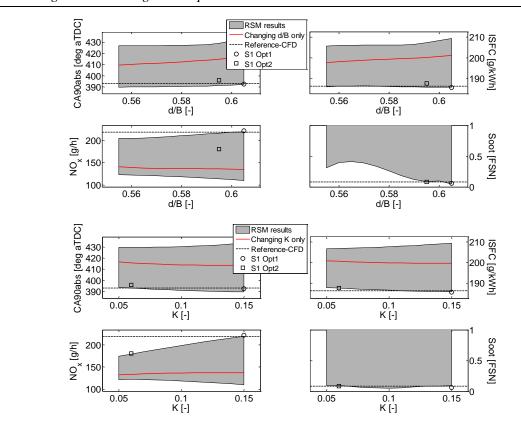


A preliminary optimization process was carried out with the aim of investigating the impact of the engine hardware and nozzle configurations on emissions and fuel consumption. This first stage focused on medium speed/load, evaluating later the optimum configurations at low speed/load and high speed/load operation conditions.

Air management and injection settings were kept constant at their reference values. Then, a double shot injection (pilot plus main events) at the reference timings and injection pressure was considered. The engine volumetric compression ratio was also kept constant at the reference value shown in Table 1.

Four parameters related to the bowl shape (diameter and re-entrant profile), intake manifold design (swirl) and injection hardware (nozzle included angle) were optimized by means of the DOE technique known as Response Surface Method. The ranges of

- these optimization parameters were shown in Table 5. Additional details of the responsesurface functions can be found in Annex 1.
- 371 Figure 9 and Figure 10 show the effects of bowl geometry (d/B and K) and the effects
- of swirl and nozzle included angle (NA) respectively on the end of combustion angle (CA90abs), engine efficiency (ISFC) and NO<sub>x</sub> -Smoke emissions.
- Focusing on the main general trends observed in Figure 9, it can be seen how increasing bowl diameter (d/B) results in a later CA90abs while the effect on ISFC is almost negligible. The impact on NO<sub>x</sub> and Smoke emissions was moderate. Additionally, increasing the reentrant shape of the bowl (K) clearly advances the end of combustion (CA90abs) and decreases ISFC independently from the combination of the other input factors. NO<sub>x</sub> emissions increase while Smoke was much less affected.
- 380 Switching to the most relevant trends observed in Figure 10, increasing swirl advances 381 CA90abs and decreases ISFC also independently from the values of the other input 382 parameters.  $NO_x$  and Smoke increase and decrease respectively. Finally, increasing the 383 nozzle included angle results in similar trends than those observed increasing swirl, so 384 wide angle nozzle provided better results in terms of ISFC and Smoke emissions.
- On the light of the results, Table 7 describes the two optimum combustion systemsdefined following two different optimization paths:
- 1. Minimizing ISFC keeping the NO<sub>X</sub>-Smoke trade-off (S1 Opt1)
- 388 2. Improving the NO<sub>x</sub> -Smoke trade-off accepting 2% ISFC penalty (S1 Opt2).
- The optimized bowl profiles compared to that of the reference combustion system are shown in Figure 11, together with the combustion system definition for those optimal configurations. Observing these data, both optimization paths resulted in similar bowl diameter, with d/B around 0.6, but higher reentrant shape, higher K, was required for the minimum ISFC criterion compared to the smaller K for the improving NO<sub>x</sub> -Smoke trade-off criterion. In all cases higher nozzle included angle than the reference engine were obtained, especially for the minimum ISFC combustion system configuration.
- 396 The two optimized configurations were modeled and compared with the reference 397 engine in Figure 12. It is shown how S1 Opt1 (best ISFC) provided slightly decreased 398 fuel consumption by less than 0.5%, while NO<sub>x</sub> slightly increases by +1.4% and the 399 Smoke level is nearly unchanged keeping FSN below 0.1. For S1 Opt 2 (best NOx -400 Smoke trade-off) NO<sub>x</sub> decreases by 17% with Smoke still below 0.1 FSN at the expense 401 of a minor increment in ISFC by 0.7%, below the acceptable limit. The two optimized 402 configurations were also evaluated for the other two operating conditions, 1800 rpm -403 high load and 1200 rpm - low load. Results shown in Figure 12 confirm that both 404 combustion systems also work adequately in these other operating conditions.

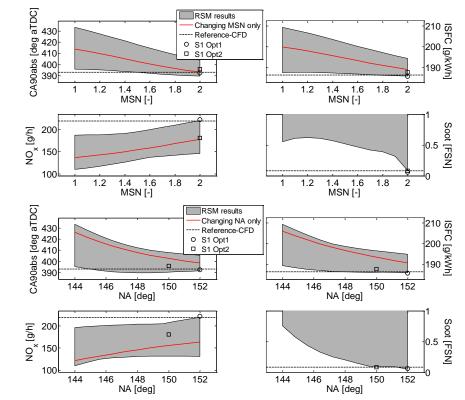






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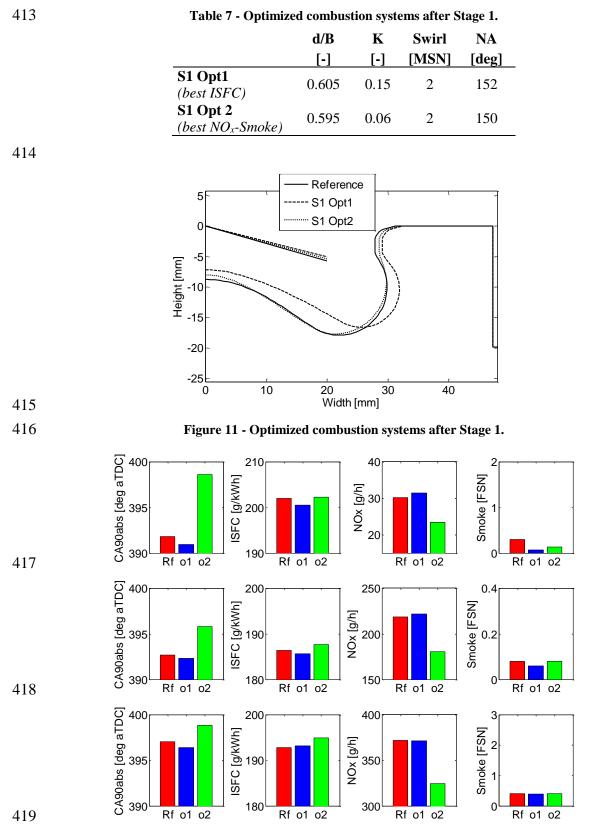
Figure 9 – Effect of d/B (top) and K (bottom) on key combustion, emissions and performance parameters. Reference engine levels are included as red lines.

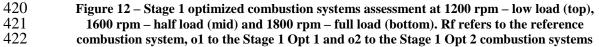


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Figure 10 - Effect of swirl (top) and Nozzle included angle (bottom) on key combustion, emissions and performance parameters. Reference engine levels are included as red lines.

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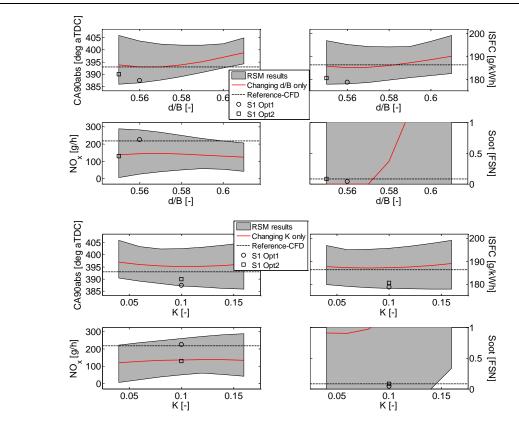
423 As a key conclusion of this Stage 1, the implementation of the original attractive 424 optimization path based on designing a quiescent combustion system with low swirl and 425 no-reentrant bowl shape, which is expected to improve engine efficiency by reducing 426 the convective heat transfer to the combustion chamber walls, was not possible at least 427 keeping the reference air management and injection settings defined by the current 428 engine technology. Additionally this Stage 1 evidences the low potential of 429 improvement in terms of ISFC while keeping constant emissions attainable by 430 optimizing only the geometry of the engine, supporting the similarity of results between 431 different geometries keeping the same injection and air management setting reported by 432 Rakopoulos et al [13]. This very limited improvement encourages the definition of a 433 second optimization stage adding the key air management (intake pressure and EGR) 434 and injection settings (start of the main injection and injection pressure) for further 435 investigating the potential for ISFC reduction.

# 436 5.3. Optimization Stage 2

437 From the knowledge generated in the previous stage, this Stage 2 focuses on defining a 438 set of optimum combustion chamber, injection settings and air management settings 439 also at the medium speed/load operating condition, evaluating the performance of the 440 optimized combustion systems in the other two operating conditions. Since the 441 maximum number of optimization parameters considered as suitable for the 442 methodology in order to have an acceptable time cost is six, and the reference nozzle 443 angle and swirl level were both quite optimized, only the two geometrical parameters 444 related to the bowl shape (d/B and K) were kept for Stage 2. The detailed information 445 about the parameters included in this optimization together with their ranges is included 446 in the methodology section (Table 6). Additional information concerning the response 447 surface functions can be found in Annex 1.

- The impact of the input parameters over the output responses was analyzed in order to establish clear cause/effect relationships. Figure 13 shows the effect of bowl geometry (d/B and K), Figure 14 the effect of air management settings (P2 and EGR) and Figure 15 the effect of injection settings (IP and SoI<sub>m</sub>) on the end of combustion angle (CA90abs), ISFC and NO<sub>x</sub>-Smoke emissions.
- Focusing on the main trends observed in Figure 13, increasing bowl diameter (d/B) clearly delays CA90abs and increases ISFC even compensating its effect by adjusting the other five input parameters. The impact on NO<sub>x</sub> and Smoke emissions is moderate and both can be easily controlled. Increasing the reentrant shape of the bowl (K) has moderate impact on CA90abs and ISFC but, contrarily to what was observed in Stage 1, now its effect can be compensated by combining properly the other input factors. NO<sub>x</sub> emissions increase while Smoke only increases for highly re-entrant bowl shapes.

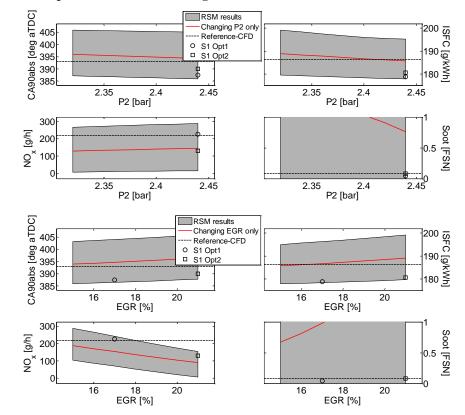
- 460 Regarding the impact of air management settings shown in Figure 14, increasing P2 461 results in a slightly earlier CA90abs and then in a reduction in ISFC independently from 462 the values of the other five input parameters. The impact on  $NO_x$  and Smoke emissions 463 is moderate and levels below those generated by the reference engine can be easily 464 attained at all P2 levels. Increasing EGR retards CA90abs and then increases ISFC but, 465 on the contrary,  $NO_x$  emissions are sharply reduced while Smoke emissions can be 466 controlled by adjusting the other parameters.
- 467 Closing this analysis by observing the effects of injection settings included in Figure 15, 468 CA90abs advances and ISFC decreases by increasing IP, and the impact on  $NO_x$  and 469 Smoke can be also minimized by adjusting the other input parameters. Advancing SoI<sub>m</sub> 470 advances CA90abs and then decreases ISFC.  $NO_x$  emissions increase while Smoke can 471 be kept at levels below the reference engine for all SoI<sub>m</sub> values.
- 472 Results confirm how the bowl shape is strongly coupled to the injector nozzle 473 configuration and, in this case, the nozzle included angle is slightly narrow (148°) and 474 then the optimized combustion systems shifts towards bowls with lower d/B values. 475 Additionally, the path for optimizing ISFC starts by advancing SoI<sub>m</sub> to decrease it 476 significantly and introducing the suitable rates of EGR in order to control NO<sub>x</sub> 477 emissions keeping a moderate impact on ISFC, while adjusting IP and P2 helps to 478 control Smoke emissions. This path fits with the current trends followed in the field of 479 diesel engine development.





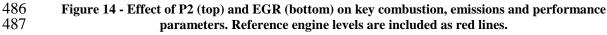


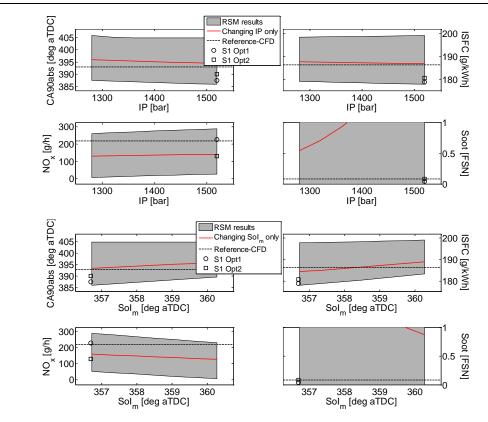
482 Figure 13 – Effect of d/B (top) and K (bottom) on key combustion, emissions and performance 483 parameters. Reference engine levels are included as red lines.





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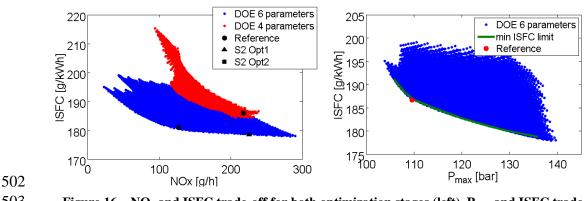


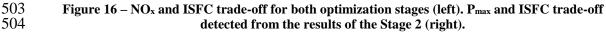
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490Figure 15 - Effect of IP (top) and SoIm (bottom) on key combustion, emissions and performance491parameters. Reference engine levels are included as red lines.

492 The NO<sub>x</sub> -ISFC trade-offs obtained after Stage 1 and Stage 2 included in Figure 16 (left) 493 show the strongly limited potential for optimization provided by modifying only the 494 geometrical parameters (Stage 1), while this potential increases significantly by 495 including the air management and injection settings (Stage 2). However, an important 496 limitation was detected after the analysis of the Stage 2 DOE related to the relation 497 between maximum cylinder pressure (P<sub>max</sub>) and ISFC observed in Figure 16 (right). It is evident how ISFC is constrained by P<sub>max</sub>, generating an additional trade-off that must be 498 499 carefully considered. In fact, the current engine ISFC level cannot be further improved 500 without increasing P<sub>max</sub> even optimizing the combustion chamber geometry and air 501 management/injection settings altogether.

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As in Stage 1, the same two optimization paths were followed for the optimization:

506 1. Minimizing ISFC keeping the NO<sub>X</sub>-Smoke trade-off (S2 Opt1)

507 2. Improving the NO<sub>x</sub> -Smoke trade-off accepting 2% ISFC penalty (S2 Opt2).

508 The combustion system definitions for those optimal configurations are included in

509 Table 8, and the bowl profiles compared to the reference combustion system and Stage

510 1 optimums are shown in Figure 17.

511

#### Table 8 - Optimized combustion systems after Stage 2

	d/B	K	P2	EGR	IP	SoIm
	[-]	[-]	[bar]	[%]	[bar]	[deg aTDC]
<b>S2 Opt1</b> (best ISFC)	0.56	0.1	2.44	17	1520	356.7
<b>S2 Opt2</b> ( <i>best NO<sub>x</sub>-Smoke</i> )	0.55	0.1	2.44	21	1520	356.7

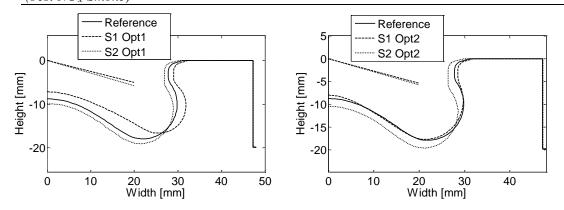






Figure 17 – Optimized piston bowl profiles best ISFC (left) and for best NO<sub>x</sub>-Smoke (right). Optimum from Stage 2 and the reference engine have the same NA.

515 In this Stage 2 the two optimization paths provided quite similar bowl geometries, with 516 d/B 0.56 for best ISFC against 0.55 for best  $NO_x$  -Smoke and K equal to 0.1 in both 517 cases. Injection settings were also similar with the highest IP of 1520 bar and the 518 earliest SoI<sub>m</sub> of 356.72° aTDC, and they even share the highest P2 equal to 2.44 bar. 519 Therefore, the key difference between both optimization paths is observed in the EGR

520 level, which shifts from 17% for the best ISFC to 21% for the best  $NO_x$  -Smoke.

521 Figure 18 compares the results of the two optimized configurations from Stage 2 with

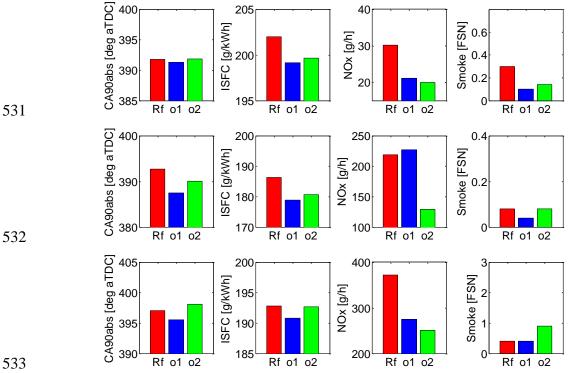
522 those obtained with the reference combustion system. According to these results, S2

523 Opt1 and S2 Opt2 decrease fuel consumption by 4.3% and by 3.2% respectively, NO<sub>x</sub>

524 slightly increases by 1% for S2 Opt1 but sharply decreases by 43% for S2 Opt2. Smoke

525 level is kept controlled at FSN levels below 0.1 in both cases.

526 As shown in Figure 18 the optimized combustion systems were also evaluated for the 527 other two operating conditions, 1800 rpm - high load and 1200 rpm - low load using the 528 specific reference setting for each case. The S2 Opt1 combustion system also works 529 adequately under high-load conditions. It is noticeable how the S2 Opt2 improves 530 further the NO<sub>x</sub> emissions and keeps a modest reduction in ISFC and soot.



534 535 536

Figure 18 - Stage 2 optimized combustion systems assessment at 1200 rpm – low load (top), 1600 rpm - half load (mid) and 1800 rpm - high load (bottom). Rf refers to the reference combustion system, o1 to the Stage 2 Opt 1 and o2 to the Stage 2 Opt 2 combustion systems

#### 537 6. Experimental validation

538 The piston geometries for both optimized combustion systems obtained using the 539 methodology described in this paper were machined and installed in the engine with the 540 aim of validating the quality of the CFD optimization results. The injection and air 541 management settings of the CFD optimums were implemented in order to replicate the

542 exact conditions for both S2 Opt1 and S2 Opt2 combustion systems. Both cases were

- 543 tested experimentally at medium speed/load and the performance was compared with
- the CFD results.

	ISFC [g/kWh]		NO <sub>x</sub> [g/h]		Soot [FSN]		dP/da [bar/deg]	
	EXP	CFD	EXP	CFD	EXP	CFD	EXP	CFD
Reference	186.3	187.8	218.6	229.8	0.08	0.08	4.2	4.3
		(-0.8%)		(+4.9%)		(+0%)		(+2.3%)
S2 Opt1	177.0	178.3	222.7	224.9	0.04	0.03	4.5	4.7
		(+0.7%)		(+1.0%)		(-33%)		(+4.3%)
S2 Opt2	178.9	180.4	152.8	146.3	0.08	0.09	4.6	4.6
		(+0.9%)		(-4.4%)		(11.1%)		(+0%)

545 Table 9 – Experimental and CFD results for S2 Opt1 and S2 Opt2 at 1600 rpm - medium load.

546 In general, the agreement is good as indicated in Table 9, confirming how the CFD 547 model setup and the optimization methodology performed well. According to the experimental results, the main objective, ISFC, was reduced by 5% and 4% with S2 548 549 Opt1 and S2 Opt2 respectively, fairly similar to the 4.3% and 3.2% predicted by the 550 CFD, while the NO<sub>x</sub> and soot were kept constant or improved compared to the 551 reference. In addition, the emission optimum, S2 Opt2, was able to reduce almost 40% 552 NO<sub>x</sub> emissions with slightly higher ISFC following also the trends predicted by CFD. 553 Finally, the pressure gradient increases by 10% in both cases, showing a possible noise 554 restriction, what was also captured accurately by the CFD except for a small 555 underprediction with the S2 Opt1.

As a result, the error between the CFD predictions and the experimental validation results is below 3% in the emissions, 2% in ISFC and 5% in noise, proving the robustness and accuracy of the new method.

559 Following the structure of the paper, the optimum bowls were evaluated at the other 560 operating conditions, 1200 rpm – low load and 1800 rpm – high load, keeping their 561 respective reference settings. However, in the particular case of 1800 rpm – high load 562 the air management and injection settings were slightly re-adjusted to fulfill the 563 mechanical restrictions of the engine along the experiments.

564 As concluded at the end of optimization Stage 1, the impact of the geometry itself on 565 ISFC is very limited, while the effect on pollutant emission levels is higher, as indicated 566 in Table 10 and Table 11. At the low load case both optimized bowls are able to reduce 567 NO<sub>x</sub> emissions by around 15%, keeping ISFC almost constant with less than a 0.5% difference. At the high load case the trend is very similar with a reduction by 6.3% NO<sub>x</sub> 568 569 for S2 Opt1 bowl and by 5% for S2 Opt2 bowl compared to the reference, together with 570 a reduction in ISFC of less than 1% for both optimized bowls. Soot emission levels 571 show little discrepancies that, due to the low value of the experimental measurements,

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572 could be explained by experimental errors and/or inaccuracies in the soot model 573 predictions. Nonetheless, the optimum bowl geometries provide competitive soot levels 574 compared to the reference bowl, even following the trends predicted by the modeling 575 results. Focusing now on pressure gradient, it increases by around 18% in the low load 576 case and by 2% in the high load case, also according with the trends previously 577 predicted.

578

Table 10 – Experimental results for S2 Opt1 and S2 Opt2 at 1200 rpm - low load.

	ISFC	NOx	Soot	dP/da
	[g/kWh]	[g/h]	[g/h]	[bar/deg]
Reference	197.72	9.52	0.04	3.92
S2 Opt1	198.23	8.07	0.03	4.79
S2 Opt2	197.52	8.18	0.05	4.5

Table 11 - Experimental results for S2 Opt1 and S2 Opt2 at 1800 rpm - high load.

	ISFC	NOx	Soot	dP/da
	[g/kWh]	[g/h]	[g/h]	[bar/deg]
Reference	181.29	103.69	0.02	4.95
S2 Opt1	179.95	94.19	0.07	5.04
S2 Opt2	179.32	98.43	0.05	5.14

As a final remark, these results confirm how the reference bowl geometry was already optimized in terms of ISFC and therefore, the potential for further improvement by reoptimizing the bowl geometry is very limited. As a consequence, air management and injection setting in addition to the bowl geometry must be included in the optimization in order to decrease ISFC by improving the combustion system.

# 585 **7. Conclusions**

586 An optimization methodology based on a combination of CFD modeling and the 587 statistical Design of Experiments (DOE) technique known as Response Surface Method 588 (RSM) was applied to a 4-cylinder 4-stroke Medium Duty Direct Injection (DI) CI 589 engine in order to reduce ISFC while keeping the main pollutants constant. This 590 methodology provided not only the optimum configurations but also the cause-effect 591 relations between the control and target parameters. This improves the understanding of 592 the requirements of the conventional diesel combustion system and what parameters are more attractive for being optimized. 593

In a first optimization stage has been found how the combustion system geometry could only improve ISFC by 0.5% without increasing NOx emissions level. This study also indicated that a swirl-supported with re-entrant bowl shape combustion system is still required for this engine and input parameter ranges.

<sup>579</sup> 

598 After that, injection and air management settings were included in order to increase the 599 potential of the optimization and to be able to significantly reduce ISFC (around 5%), for constant NO<sub>x</sub> emissions, as confirmed by the second optimization stage. It is also 600 601 noticeable that 40% NO<sub>x</sub> reduction can be obtained keeping constant ISFC and soot emissions. Optimization path leads to advanced SoI for improved ISFC, increased EGR 602 in order to control NO<sub>x</sub> emissions keeping a moderate impact on ISFC, while adjusting 603 604 IP and P2 helps to control soot emissions. This path fits with the current trends followed 605 in the field of diesel engine development. 606

607	Ref	ferences
608	1.	CHOI, S.; SHIN, S.; LEE, J.; MIN, K.; CHOI, H. The effects of the combustion chamber
609		geometry and a double-row nozzle on the diesel engine emissions. Proceedings of the
610		Institution of Mechanical Engineers, Part D: Journal of Automobile Engineering, 2015, vol.
611		229, no 5, p. 590-598.
612	2.	ATMANLI, A.; YÜKSEL, B.; ILERI, E.; KARAOGLAN, A. D. Response surface
613		methodology based optimization of diesel-n-butanol-cotton oil ternary blend ratios to
614		improve engine performance and exhaust emission characteristics. Energy Conversion and
615		Management, 2015, vol. 90, p. 383-394.
616	3.	GENZALE, C. L.; REITZ, R. D.; MUSCULUS, M. PB. Effects of piston bowl geometry on
617		mixture development and late-injection low-temperature combustion in a heavy-duty diesel
618		engine. SAE Technical Paper, 2008.
619	4.	BENAJES, J.; PASTOR, J.V.; GARCÍA, A.; MONSALVE-SERRANO, J. An
620		experimental investigation on the influence of piston bowl geometry on RCCI performance
621		and emissions in a heavy-duty engine. Energy Conversion and Management, 2015, vol.
622		103, p. 1019-1030.
623	5.	PARK, S. W. Optimization of combustion chamber geometry for stoichiometric diesel
624		combustion using a micro genetic algorithm. Fuel Processing Technology, 2010, vol. 91,
625		no 11, p. 1742-1752.
626	6.	WICKMAN, D. D.; YUN, H.; REITZ, R. D. Split-spray piston geometry optimized for
627		HSDI diesel engine combustion. SAE Technical Paper, 2003.
628	7.	SHI, Y.; REITZ, R. D. Optimization of a heavy-duty compression-ignition engine fueled
629		with diesel and gasoline-like fuels. Fuel, 2010, vol. 89, no 11, p. 3416-3430.
630	8.	KIM, D.; PARK, S Optimization of injection strategy to reduce fuel consumption for
631		stoichiometric diesel combustion. Fuel, 2012, vol. 93, p. 229-237.
632	9.	SUN, Y.; REITZ, R. D. Modeling diesel engine $NO_x$ and soot reduction with optimized
633		two-stage combustion. SAE Technical Paper, 2006.
634	10.	KOKJOHN, S. L.; REITZ, R. D. A computational investigation of two-stage combustion in
635		a light-duty engine. SAE Technical Paper, 2008.
636	11.	GAFOOR, CP A.; GUPTA, R Numerical investigation of piston bowl geometry and swirl
637		ratio on emission from diesel engines. Energy Conversion and Management, 2015, vol.
638		101, p. 541-551.
639	12.	GE, H.; SHI, Y.; REITZ, R.; WICKMAN, D.; WILLEMS, W. Engine development using
640		multi-dimensional CFD and computer optimization. SAE Technical Paper, 2010.
641	13.	RAKOPOULOS, C. D.; KOSMADAKIS, G. M.; PARIOTIS, E. G. Investigation of piston
642		bowl geometry and speed effects in a motored HSDI diesel engine using a CFD against a
643		quasi-dimensional model. Energy Conversion and Management, 2010, vol. 51, no 3, p.
644		470-484.
645	14.	YUN, H.; REITZ, R. D. An experimental study on emissions optimization using micro-
646		genetic algorithms in a HSDI diesel engine. SAE Technical Paper, 2003.
647	15.	KIM, M.; LIECHTY, M. P.; REITZ, R. D. Application of micro-genetic algorithms for the
648		optimization of injection strategies in a heavy-duty diesel engine. SAE Technical Paper,
649		2005.
650	16.	SHI, Y; REITZ, R. D. Assessment of optimization methodologies to study the effects of
651		bowl geometry, spray targeting and swirl ratio for a heavy-duty diesel engine operated at
652		high-load. SAE Technical Paper, 2008.
653	17.	SHI, Y.; GE, H.; REITZ, R. D. Computational optimization of internal combustion
654		engines. Springer Science & Business Media, 2011.

- 18. HAJIREZA, S.; REGNER, G.; CHRISTIE, A.; EGERT, M.; MITTERMAIER, H. *Application of CFD modeling in combustion bowl assessment of diesel engines using DoE methodology*. SAE Technical Paper, 2006.
- YUAN, Y.; LI, G. X.; YU, Y. S.; ZHAO, P.; LI, H. M. Multi-Parameter and Multi-Object *Optimization on Combustion System of High Power Diesel Engine Based on Response Surface Method.* Chinese Internal Combustion Engine Engineering, 2012, vol. 5, p. 005.
- REITZ, R.; VON DER EHE, J. Use of in-cylinder pressure measurement and the response *surface method for combustion feedback control in a diesel engine*. Proceedings of the
  Institution of Mechanical Engineers, Part D: Journal of Automobile Engineering, 2006, vol.
  220, no 11, p. 1657-1666.
- LEE, T.; REITZ, R. D. Response surface method optimization of a high-speed directinjection diesel engine equipped with a common rail injection system. Journal of engineering for gas turbines and power, 2003, vol. 125, no 2, p. 541-546.
- LAPUERTA, M.; ARMAS, O.; HERNÁNDEZ, J. J. Diagnosis of DI Diesel combustion *from in-cylinder pressure signal by estimation of mean thermodynamic properties of the gas.* Applied Thermal Engineering, 1999, vol. 19, no 5, p. 513-529.
- 671 23. PAYRI, F.; MOLINA, S.; MARTÍN, J.; ARMAS, O. Influence of measurement errors and
  672 estimated parameters on combustion diagnosis. Applied Thermal Engineering, 2006, vol.
  673 26, no 2, p. 226-236.
- 674 24. BOSCH, W. The fuel rate indicator: a new measuring instrument for display of the
  675 characteristics of individual injection. SAE Technical Paper, 1966.
- 676 25. METHODOLOGY, STAR-CD. Version 4.18. 2012.
- 677 26. COLIN, O.; BENKENIDA, A. *The 3-zones extended coherent flame model (ECFM3Z) for*678 *computing premixed/diffusion combustion*. Oil & Gas Science and Technology, 2004, vol.
  679 59, no 6, p. 593-609.
- 680 27. KARLSSON, A.; MAGNUSSON, I.; BALTHASAR, M.; MAUSS, F. Simulation of soot
  681 formation under diesel engine conditions using a detailed kinetic soot model. SAE
  682 Technical Paper, 1998.
- 683 28. HIROYASU, H.; KADOTA, T. Models for combustion and formation of nitric oxide and
  684 soot in direct injection diesel engines. SAE Technical Paper, 1976.
- 685 29. HUH, K. Y.; GOSMAN, A. D. A phenomenological model of diesel spray atomization. In
  686 Proceedings of the international conference on multiphase flows. 1991.
- 687 30. REITZ, R. D.; DIWAKAR, R. Structure of high-pressure fuel sprays. SAE Technical
  688 Paper, 1987.
- 689 31. HABCHI, C.; LAFOSSAS, F. A.; BÉARD, P.; BROSETA, D. Formulation of a one690 component fuel lumping model to assess the effects of fuel thermodynamic properties on
  691 internal combustion engine mixture preparation and combustion. SAE Technical Paper,
  692 2004.
- 32. YAKHOT, V.; ORSZAG, S. A. *Renormalization group analysis of turbulence. I. Basic theory.* Journal of scientific computing, 1986, vol. 1, no 1, p. 3-51.
- ANGELBERGER, C.; POINSOT, T.; DELHAY, B. Improving near-wall combustion and
   wall heat transfer modeling in SI engine computations. SAE Technical Paper, 1997.
- 697 34. ISSA, R. I. Solution of the implicitly discretised fluid flow equations by operator-splitting.
  698 Journal of computational physics, 1986, vol. 62, no 1, p. 40-65.

# 700 NOMENCLATURE

701	aTDC	After Top Dead Center
702	BDC	Bottom Dead Center
703	CA50	Crank angle for 50% of fuel burnt
704	CA90	Crank angle for 90% of fuel burnt
705	CA90ab	
706	CALME	
707	CCD	Central Composite Design
708	CI	Compression Ignition
709	CFD	Computational Fluid Dynamics
710	d/B	Ratio between the rip bowl diameter (d) and the piston bore (B)
711	DI	Direct Injection
712	DOE	Design of Experiments
713	EGR	Exhaust Gas Recirculation
714	EVO	Exhaust Valve Opening (angle)
715	Exp	Experimental
716	FSN	Filter Smoke Number
717	HRR	Heat Release Rate
718	ICE	Internal Combustion Engines
719	IMEP	Indicated Mean Effective Pressure
720	IP	Injection Pressure
721	IRDCI	Injection Rate Discharge Curve Indicator
722	ISFC	Indicated specific fuel consumption
723	IVC	Intake Valve Closing (angle)
724	Κ	Geometric parameter to control the reentrant shape of the bowl
725	LTC	Low Temperature Combustion
726	m	Mass
727	MARS	Monotone Advection and Reconstruction
728	MSN	Mean Swirl Number
729	NA	Nozzle angle
730	Opt1	Optimum number 1
731	Opt2	Optimum number 2
732	P	Pressure
733	P2	Intake pressure
734	PISO	Pressure Implicit with Splitting Operators
735	P <sub>IVC</sub>	Pressure at IVC
736	P <sub>max</sub>	Maximum Cylinder Pressure
737	RCCI	Reactivity Controlled Compression Ignition
738	RSM	Response Surface Methods
739	SoI <sub>m</sub>	Start of Main Injection
740	Т	Temperature
741	TDC	Top Dead Centre
742	T <sub>wpis</sub>	Mean Temperature of the piston
743	T <sub>wliner</sub>	Mean Temperature of the liner
744	Twhead	Mean Temperature of the head
745	YO <sub>2</sub>	Oxygen concentration in the cylinder
746	$YN_2$	Nitrogen concentration in the cylinder
747	YCO <sub>2</sub>	$CO_2$ concentration in the cylinder
748	YH <sub>2</sub> O	H <sub>2</sub> O concentration in the cylinder
749		·

# 750 Annex 1- Response surfaces functions

#### 751 752

The mathematical model used to correlate the optimized input and the outputs of theStage 1 are shown below.

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 $\begin{array}{ll} 756 & Output = C_1 + db^*C_2 + k^*C_3 + MSN^*C_4 + NA^*C_5 + db^{2*}C_6 + k^{2*}C_7 + MSN^{2*}C_8 + \\ 757 & NA^{2*}C_9 + db^*MSN^*C_{10} + db^*k^*C_{11} + db^*NA^*C_{12} + k^*MSN^*C_{13} + k^*NA^*C_{14} + \\ 758 & MSN^*NA^*C_{15} + db^*k^*MSN^*C_{16} + db^*k^*NA^*C_{17} + k^*MSN^*NA^*C_{18} + \\ 759 & db^*MSN^*NA^*C_{19} + db^*k^*MSN^*NA^*C_{20} + MSN^{3*}C_{21} + db^{3*}C_{22} + NA^3 + C_{23} \\ \end{array}$ 

761 Where the inputs db, k, MSN and NA as calculated as the example below.

763  $db = (db_{value} - (db_{max} + db_{min}) / 2) / ((db_{max} - db_{min}) / 2)$ 

being  $db_{value}$  the value of db that want to be calculated,  $db_{max}$  the maximum value of db in the range used for the optimization and  $db_{min}$  the minimum value of db in the range used for the optimization.

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The coefficients C1 to C23 are described in Table 12.

Table 12 RSM coefficients for the Stage 1 optimization.

	Mathematical fit coefficients								
Output	P <sub>max</sub>	dP/da	NO <sub>x</sub>	Smoke	ISFC	CA90abs			
<b>C</b> <sub>1</sub>	106.645	4.277	160.159	2.911	192.207	398.306			
C <sub>2</sub>	0.809	0.030	5.365	-0.118	0.367	2.625			
C <sub>3</sub>	1.321	0.005	27.339	-0.806	-2.668	-4.482			
<b>C</b> <sub>4</sub>	1.438	-0.064	38.838	-4.533	-9.701	-18.410			
C₅	0.421	0.003	29.962	-3.121	-8.638	-13.717			
C <sub>6</sub>	0.513	0.014	3.692	-0.069	0.035	3.724			
C <sub>7</sub>	1.134	0.016	-8.132	0.659	1.392	4.845			
C <sub>8</sub>	0.132	0.006	12.259	-0.169	-0.079	3.014			
C <sub>9</sub>	0.193	0.031	-14.017	1.293	6.670	17.469			
C <sub>10</sub>	1.547	0.041	7.776	-0.485	-2.338	-3.830			
C <sub>11</sub>	-0.523	-0.007	-27.225	2.281	4.958	7.690			
C <sub>12</sub>	0.464	-0.037	23.413	-0.537	-4.443	-8.081			
C <sub>13</sub>	1.462	0.001	17.723	2.436	1.411	2.702			
C <sub>14</sub>	1.278	-0.034	38.268	-1.751	-3.512	-3.262			
C <sub>15</sub>	-1.166	0.016	-21.264	3.060	10.073	19.932			
C <sub>16</sub>	0.023	-0.022	-6.944	0.733	-1.686	-4.781			

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C <sub>17</sub>	0.030	-0.020	13.047	-2.269	-3.828	-8.712
C <sub>18</sub>	-0.586	0.011	-14.584	1.698	1.479	0.082
C <sub>19</sub>	-0.378	0.005	21.693	-0.588	0.884	5.400
C <sub>20</sub>	-0.156	-0.040	49.228	-5.027	0.929	4.656
C <sub>21</sub>	-	-	-12.957	1.496	5.349	10.925
C <sub>22</sub>	-	-	-18.227	2.481	3.684	3.728
C <sub>23</sub>	-	-	-4.325	-0.451	-2.468	-6.683

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 Table 13 Pvalue for all the coefficients used in the RSM for Stage 1

from the ANOVA for each coefficient is shown in Table 13.

A study of the significance level of the coefficients was performed. The results obtained

	Pvalues for all coefficients							
Output	P <sub>max</sub>	dP/da	NO <sub>x</sub>	Smoke	ISFC	CA90abs		
C1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000		
C <sub>2</sub>	0.0050	0.0020	0.2764	0.0542	0.0501	0.0432		
C <sub>3</sub>	0.0000	0.0579	0.0031	0.2592	0.0442	0.0328		
C4	0.0000	0.0000	0.0012	0.0007	0.0160	0.0003		
<b>C</b> <sub>5</sub>	0.0036	0.1753	0.0028	0.0012	0.0118	0.0001		
C <sub>6</sub>	0.0095	0.0046	0.0182	0.0656	0.6413	0.6588		
C <sub>7</sub>	0.0068	0.0698	0.0002	0.0226	0.3081	0.5701		
C <sub>8</sub>	0.0001	0.0072	0.3220	0.0186	0.0386	0.0689		
C <sub>9</sub>	0.0000	0.2239	0.0159	0.2703	0.0198	0.1567		
C <sub>10</sub>	0.0002	0.0045	0.4115	0.6025	0.0063	0.1781		
C <sub>11</sub>	0.0207	0.4582	0.0258	0.4750	0.0298	0.0031		
C <sub>12</sub>	0.0318	0.0071	0.0430	0.5656	0.0332	0.0260		
C <sub>13</sub>	0.0002	0.9531	0.0967	0.0384	0.1038	0.3432		
C <sub>14</sub>	0.0005	0.0101	0.0070	0.1011	0.0420	0.2622		
C <sub>15</sub>	0.0007	0.1135	0.0580	0.0172	0.0147	0.0006		
C <sub>16</sub>	0.8189	0.4682	0.8249	0.6217	0.1711	0.0371		
C <sub>17</sub>	0.7649	0.5000	0.6897	0.8537	0.0769	0.2885		
C <sub>18</sub>	0.1299	0.8362	0.6595	0.5325	0.3079	0.1662		
C <sub>19</sub>	0.0845	0.6659	0.5401	0.8495	0.1938	0.2591		
C <sub>20</sub>	0.4563	0.6451	0.0168	0.7431	0.0088	0.6117		
C <sub>21</sub>	-	-	0.1891	0.0303	0.8195	0.5569		
C <sub>22</sub>	-	-	0.032	0.3963	0.06325	0.0042		

C <sub>23</sub>	-	-	0.7656	0.2488	0.0062	0.8537

781 All the coefficient shown in Table 13 proved to be significant at least for one of the 782 outputs studied in this paper so as a matter of simplifying the calculations, they were all 783 kept. In order to show the fit of the surfaces compared to the original data, Table 14 784 shows the  $R^2$  values.

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### Table 14 R<sup>2</sup> values for the surfaces obtained for every output in Stage 1

Output	P <sub>max</sub>	dP/da	NO <sub>x</sub>	Smoke	ISFC	CA90abs
R <sup>2</sup>	0.9888	0.9409	0.9918	0.9838	0.9975	0.9986

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790 It can be seen that, except for the pressure gradient that shows a lower fitting level than 791 the other, all the surfaces can accurately predict the values of the original DOE points. 792

793 The mathematical model used to correlate the optimized input and the outputs of the 794 Stage 2 are shown below.

796 Output =  $C_1 + db^*C_2 + k^*C_3 + P2^*C_4 + EGR^*C_5 + IP^*C_6 + SoI_m^*C_7 + db^{2*}C_8 + k^{2*}C_9$ 797  $+ P2^{2*}C_{10} + EGR^{2*}C_{11} + IP^{2*}C_{12} + SoI_m^{2*}C_{13} + P2^{*}IP^{*}C_{14} + P2^{*}EGR^{*}C_{15} + P2^{*}IP^{*}C_{14} + P2^{*}EGR^{*}C_{15} + P2^{*}IP^{*}C_{14} + P2^{*}EGR^{*}C_{15} + P2^{*}IP^{*}C_{14} + P2^{*}EGR^{*}C_{15} + P2^{*}IP^{*}C_{16} + P2^{*}IP^{*}C_{16$ 798  $P2*SoI_m*C_{16} + P2*db*C_{17} + P2*k*C_{18} + EGR*IP*C_{19} + EGR*SoI_m*C_{20} + EGR*db$ 799  $*C_{21} + EGR*k*C_{22} + IP*SoI_m*C_{23} + IP*db*C_{24} + IP*k*C_{25} + SoI_m*db*C_{26} + IP*k*C_{25} + SoI_m*db*C_{26} + IP*K*C_{25} + IP*K*C_{25} + IP*K*C_{26} + IP*K$  $SoI_{m}*k*C_{27}+db*k*C_{28}+db^{3*}C_{29}+k^{3*}C_{30}+P2^{3*}C_{31}+EGR^{3*}C_{32}+MSN^{3*}C_{33}+harrow C_{33}+harrow C_{33$ 800 801  $SoI_{m}^{-3}*C_{34} + db2*k*C_{35} + db*IP*P2*C_{36} + db*k*P2*C_{37} + db*k*EGR*C_{38} + db*k*C_{38} + db*k*EGR*C_{38$  $db*k*IP*C_{39} + db*k*SoI_m*C_{40} + EGR*IP*SoI_m*C_{41} + EGR*P2*k*C_{42} + db2*P2*C_{43} + C_{44} + C_{44}$ 802  $+ P2*IP*k*C_{44} + P2*IP*SoI_m*C_{45} + P2*k*SoI_m*C_{46} + db2*k2*C_{47} + D2*k*SoI_m*C_{46} + db2*k2*C_{47} + D2*k*C_{47} + D2*k*C_{46} + db2*k*C_{47} + D2*k*C_{46} + db2*k*C_{47} + D2*k*C_{46} + db2*k*C_{47} + D2*k*C_{47} + D2*k*C_{46} + db2*k*C_{47} + D2*k*C_{47} + D2*k*C_{47$ 803 804  $db*k*IP*SoI_m*C_{48} + db*k*IP*P2*C_{49} + db*k*IP*EGR*C_{50}$ 805 806 807 Where the inputs db, k, P2, EGR, IP and SoI<sub>m</sub> as calculated as the example below. 808 809  $db = (db_{value} - (db_{max} + db_{min}) / 2) / ((db_{max} - db_{min}) / 2)$ 810 The coefficients  $C_1$  to  $C_{50}$  are described in Table 15.

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#### Table 15 RSM coefficients for the Stage 2 optimization.

	Mathematical fit coefficients								
Output	$P_{max}$	dP/da	NO <sub>x</sub>	Smoke	ISFC	CA90abs			
<b>C</b> <sub>1</sub>	120.017	4.454	149.017	0.485	185.110	393.201			
C <sub>2</sub>	0.016	-0.040	-29.074	4.132	5.690	6.148			
C <sub>3</sub>	2.220	-0.022	24.229	0.284	0.186	-1.707			
C <sub>4</sub>	4.323	0.122	12.870	-0.294	-2.336	-1.322			
C <sub>5</sub>	-2.108	-0.150	-90.032	0.745	2.467	2.076			

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C <sub>6</sub>	3.742	0.110	12.108	0.817	-0.892	-1.576
C <sub>7</sub>	-16.124	0.007	-31.926	-0.698	4.501	2.818
C <sub>8</sub>	-0.793	0.056	-35.064	2.079	5.223	7.165
C <sub>9</sub>	-0.290	0.054	-26.282	1.487	3.123	4.153
C <sub>10</sub>	-0.093	0.051	-2.743	0.432	0.190	0.037
C <sub>11</sub>	-0.190	0.060	6.215	0.292	0.348	0.229
C <sub>12</sub>	-0.115	0.051	-2.924	0.117	0.156	0.191
C <sub>13</sub>	2.105	0.032	1.256	0.610	0.571	0.088
C <sub>14</sub>	0.061	-0.006	1.561	0.084	-0.053	-0.031
C <sub>15</sub>	0.100	-0.031	0.401	-0.179	-0.528	-0.306
C <sub>16</sub>	-0.540	0.008	-3.760	0.120	0.070	0.035
C <sub>17</sub>	0.191	0.003	1.728	-1.926	-1.543	-0.728
C <sub>18</sub>	-0.041	-0.019	3.879	0.152	-0.527	-0.487
C <sub>19</sub>	-0.302	0.039	-5.705	0.021	-0.099	-0.160
C <sub>20</sub>	0.414	0.001	10.982	-0.117	0.072	0.089
C <sub>21</sub>	0.506	-0.032	17.965	1.574	1.045	0.223
C <sub>22</sub>	-0.321	-0.016	-9.766	0.149	0.113	-0.054
C <sub>23</sub>	-0.772	-0.016	-1.329	0.126	-0.507	-0.232
C <sub>24</sub>	-1.044	-0.029	-14.468	2.219	1.923	1.240
C <sub>25</sub>	0.780	-0.003	-3.073	-0.584	1.119	1.162
C <sub>26</sub>	0.631	-0.001	20.299	-2.074	-2.873	-2.897
C <sub>27</sub>	-0.129	-0.005	6.356	0.021	-2.061	-1.948
C <sub>28</sub>	-2.940	-0.010	-65.452	4.177	7.212	8.576
C <sub>29</sub>	2.071	0.011	36.321	-2.335	-4.346	-4.082
C <sub>30</sub>	-0.529	0.008	-5.271	1.339	-0.564	-0.674
C <sub>31</sub>	0.008	0.015	3.204	-0.506	-0.009	0.024
C <sub>32</sub>	0.142	0.010	8.861	-0.057	-0.003	0.000
C <sub>33</sub>	-0.413	0.031	-0.448	-0.435	-0.007	0.148
C <sub>34</sub>	2.327	-0.021	0.582	-0.256	-0.368	-0.221
C <sub>35</sub>	-	-	-	7.720	-	-
C <sub>36</sub>	-	-	-	0.310	-	-
C <sub>37</sub>	-	-	-	0.759	-	-
C <sub>38</sub>	-	-	-	0.223	-	-
C <sub>39</sub>	-	-	-	-2.115	-	-
C <sub>40</sub>	-	-	-	0.979	-	-
C <sub>41</sub>	-	-	-	0.354	-	-

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C <sub>42</sub>	-	-	-	0.406	-	-
C <sub>43</sub>	-	-	-	-2.684	-	-
C <sub>44</sub>	-	-	-	0.488	-	-
C <sub>45</sub>	-	-	-	-0.587	-	-
C <sub>46</sub>	-	-	-	-0.653	-	-
C <sub>47</sub>	-	-	-	1.517	-	-
C <sub>48</sub>	-	-	-	25.523	-	-
C <sub>49</sub>	-	-	-	1.793	-	-
C <sub>50</sub>	-	-	-	-2.335	-	-

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Table 16 P-value for all the coefficients used in the RSM for Stage 2

ANOVA for each coefficient is shown in Table 16.

A study of the significance level of the coefficients was performed. The results from the

			P-values for	all coefficien	ts	
Output	P <sub>max</sub>	dP/da	NO <sub>x</sub>	Smoke	ISFC	CA90abs
C1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
C <sub>2</sub>	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
C <sub>3</sub>	0.0000	0.0091	0.0000	0.0000	0.0000	0.0000
C4	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
C <sub>5</sub>	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
C <sub>6</sub>	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
C <sub>7</sub>	0.0000	0.0230	0.0000	0.0000	0.0000	0.0000
C <sub>8</sub>	0.5700	0.6420	0.0398	0.4825	0.0747	0.0127
C <sub>9</sub>	0.1705	0.2001	0.0329	0.5237	0.0000	0.0185
C <sub>10</sub>	0.6505	0.5300	0.0000	0.3154	0.0000	0.1019
C <sub>11</sub>	0.0245	0.5276	0.2360	0.0587	0.5424	0.0000
C <sub>12</sub>	0.1376	0.2663	0.1135	0.0000	0.5721	0.6085
C <sub>13</sub>	0.0176	0.3975	0.0556	0.6393	0.6081	0.4058
C <sub>14</sub>	0.1405	0.9186	0.0000	0.6269	0.2372	0.0011
C <sub>15</sub>	0.0309	0.0329	0.0575	0.3139	0.0000	0.0000
C <sub>16</sub>	0.0000	0.6125	0.0000	0.4784	0.1610	0.0001
C <sub>17</sub>	0.0013	0.6125	0.0000	0.0000	0.0000	0.0000
C <sub>18</sub>	0.3005	0.1559	0.0000	0.3973	0.0000	0.0000
C <sub>19</sub>	0.0001	0.0243	0.0000	0.8713	0.0664	0.5043
C <sub>20</sub>	0.0000	0.7598	0.0000	0.5138	0.1373	0.0021
C <sub>21</sub>	0.0000	0.0613	0.0000	0.0000	0.0000	0.0000

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C <sub>22</sub>	0.0001	0.2106	0.0000	0.3973	0.0443	0.0000
C <sub>23</sub>	0.0000	0.2818	0.0001	0.4613	0.0000	0.0001
C <sub>24</sub>	0.0000	0.0449	0.0000	0.0000	0.0000	0.0000
C <sub>25</sub>	0.0000	0.7598	0.0000	0.0092	0.0000	0.0000
C <sub>26</sub>	0.0000	0.9186	0.0000	0.0000	0.0000	0.0000
C <sub>27</sub>	0.0103	0.7598	0.0000	0.8945	0.0000	0.0000
C <sub>28</sub>	0.0000	0.2818	0.0000	0.0000	0.0000	0.0000
C <sub>29</sub>	0.0431	0.0531	0.2179	0.1067	0.0591	0.3849
C <sub>30</sub>	0.3313	0.0378	0.0370	0.5781	0.2798	0.1015
C <sub>31</sub>	0.2462	0.3716	0.1160	0.3768	0.0182	0.5971
C <sub>32</sub>	0.5816	0.5454	0.4214	0.6973	0.5600	0.0435
C <sub>33</sub>	0.0410	0.6538	0.0184	0.0547	0.3020	0.2457
C <sub>34</sub>	0.3848	0.0909	0.0458	0.3099	0.6375	0.3593
C <sub>35</sub>				0.0081		
C <sub>36</sub>				0.0522		
C <sub>37</sub>				0.0142		
C <sub>38</sub>				0.0063		
C <sub>39</sub>				0.0026		
C <sub>40</sub>				0.0463		
C <sub>41</sub>				0.0469		
C <sub>42</sub>				0.0421		
C <sub>43</sub>				0.0021		
C <sub>44</sub>				0.0333		
<b>C</b> 45				0.025		
C <sub>46</sub>				0.0194		
C <sub>47</sub>				0.1311		
C <sub>48</sub>				0.0289		
C <sub>49</sub>				0.021		
C <sub>50</sub>				0.011		

All the coefficient shown in Table 16 proved to be significant at least for one of the
outputs studied in this paper so as a matter of simplifying the calculations, they were all
kept. In order to show the fit of the surfaces compared to the original data, Table 17
shows the R<sup>2</sup> values.

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830 831	Table 17 R <sup>2</sup> values for the surfaces obtained for every output in Stage 1									
	Output	$P_{max}$	dP/da	NO <sub>x</sub>	Smoke	ISFC	CA90abs			
	R <sup>2</sup>	0.9981	0.9597	0.998	0.9904	0.9978	0.9934			

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833 It can be seen that, except for the pressure gradient that shows a lower fitting level than

the other, all the surfaces can accurately predict the values of the original DOE points.

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