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1 A RANS Knock Model to Predict the Statistical Occurrence of Engine 2 Knock

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16 Abstract

17 In the recent past engine knock emerged as one of the main limiting aspects for the achievement of higher
18 efficiency targets in modern spark-ignition (SI) engines. To attain these requirements, engine operating
19 points must be moved as close as possible to the onset of abnormal combustions, although the turbulent
20 nature of flow field and SI combustion leads to possibly ample fluctuations between consecutive engine
21 cycles. This forces engine designers to distance the target condition from its theoretical optimum in order to
22 prevent abnormal combustion, which can potentially damage engine components because of few individual
23 heavy-knocking cycles.

24 A statistically based RANS knock model is presented in this study, whose aim is the prediction not only of
25 the ensemble average knock occurrence, poorly meaningful in such a stochastic event, but also of a knock
26 probability. The model is based on look-up tables of autoignition times from detailed chemistry, coupled
27 with transport equations for the variance of mixture fraction and enthalpy. The transported perturbations
28 around the ensemble average value are based on variable gradients and on a local turbulent time scale. A
29 multi-variate cell-based Gaussian-PDF model is proposed for the unburnt mixture, resulting in a statistical
30 distribution for the in-cell reaction rate. An average knock precursor and its variance are independently
31 calculated and transported; this results in the prediction of an earliest knock probability preceding the
32 ensemble average knock onset, as confirmed by the experimental evidence. The proposed model estimates
33 not only the regions where the average knock is promoted, but also where and when the first knock is more
34 likely to be encountered.

35 The application of the model to a RANS simulation of a modern turbocharged direct injection (DI) SI engine
36 with optical access is presented and the analysis of the knock statistical occurrence obtained by the proposed
37 model adds an innovative contribution to overcome the limitation of consolidated "average knock" analyses
38 typical of a RANS approach.

39

40 Introduction

41 In the last decades several approaches were proposed to numerically predict and simulate the average engine
42 knock in the framework of RANS simulations. Their development was driven to meet the increasing
43 efficiency targets requested by legislation. Thermal efficiency and specific output power are raised to
44 unprecedented levels, in order both to reduce fuel consumption and pollutant emissions and to
45 simultaneously preserve the desired target performance levels.

46 Under high thermal loads abnormal combustion events are promoted, the most harmful of which is engine
47 knock. Knock is the consequence of the self-ignition of a portion of unburnt mixture ahead of the main
48 propagating flame front, and its occurrence is enhanced by the mentioned strategies, as outlined in [1]. Given
49 the need to operate as close as possible to the theoretical optimum of the regular combustion range [2] and
50 the simultaneous random nature of the turbulent combustion typical of internal combustion engines, the
51 occurrence of engine knock is a possibility that is always to be accounted for when the operating condition is
52 experimentally calibrated. To this aim, in-cylinder pressure is monitored in order to observe the random
53 presence of knocking events. This is assessed by the definition of knock indices, such as the commonly
54 adopted MAPO (Maximum Amplitude of Pressure Oscillations) or IMPO (Integral Modulus of Pressure
55 Oscillations) as widely surveyed by [3, 4, 5], as well as other indicators like the DKI (Dimensionless Knock
56 Indicator) [6] or the time-derivative of the in-cylinder pressure trace. Irrespectively of the chosen indicator,
57 an arbitrary threshold value is always present to discern between a soft and acceptable knock intensity and a
58 heavy and damaging knock level. Threshold values are part of engine manufacturer know-how and
59 standardized limits are not defined.

60 All the mentioned aspects motivate why a significant research effort was paid to knock prediction in the
61 recent years. Quasi-dimensional and three-dimensional CFD models for average knock prediction were
62 developed and validated against experiments by several research groups. Vancoillie and co-authors used a
63 fuel-specific Arrhenius formulation for the reaction rate of methanol and ethanol fuels in [7], and the average
64 ignition delay was used to integrate a knock precursor species. A similar modelling approach was used by
65 Forte et al. [8] and Corti et al. in [9] for gasoline fuels.

66 However, the ensemble average approach to knock modelling through the use of RANS simulations suffers
67 of the inability to reproduce the intrinsically stochastic nature of knock; this is a strong limitation for this
68 type of models. The dramatic impact of cycle-to-cycle variability (CCV) on all the in-cylinder physical
69 processes, such as fuel-air mixing, combustion initiation and turbulent burn rate, motivates the adoption of
70 more refined approaches. In fact, since engine knock depends on all the preceding processes, it is itself a
71 typically stochastic and cycle-dependent phenomenon whose accurate prediction is therefore extremely
72 complex. A rigorous analysis of CCV can only be carried out through the use of Large-Eddy Simulation
73 (LES), where the largest flow structures are resolved allowing the simulation of flow unsteadiness deriving
74 from large-scale turbulence. Despite the still demanding cost of this type of analyses, several promising
75 studies of this kind were presented in the recent years, such as the works by Robert et al. [10, 11]. They
76 showed that the simulated combustion CCV was able to replicate the degree on instability measured at the
77 test-bench for a premixed isoctane-air engine at several spark timings. Large-Eddy Simulation was used to
78 predict knock occurrence in a turbocharged GDI unit by the authors in previous studies [12, 13, 14], and the
79 cycle-dependent knock-signature well correlated with the outcomes from the experimental test-bench for
80 both Knock-Limited Spark Advance (KLSA) and for a knocking regime with an advanced spark-timing.
81 These examples showed the investigation insight made possible by LES and the possibility to explain
82 individual misfiring cycles or cycle-specific knocking events, thus allowing a direct comparison between
83 simulation results and engine test-bench output. However, the application of LES on production engines still
84 suffers from the severe computational cost, preventing a full application in the design process of current
85 units.

86 In this context the definition of a new approach for knock modelling emerges as a necessary bridge between
87 the poorly representative RANS mean knock prediction and the relevant CPU effort of a multiple cycle LES
88 study. This is based on the RANS formalism for average quantities, combined with the use of transport
89 equations for variances of physical conditions, allowing to estimate a knock probability or a fraction of
90 knocking cycles. The statistical RANS knock model proposed in this paper relies on transport equations for
91 mixture fraction and enthalpy variances; detailed chemistry is used to calculate an accurate ignition delay of
92 a gasoline surrogate model for the unburnt mixture. The variances of the variable are used as a basis of a
93 multi-variate Gaussian model of the unburnt fluid cell, from which information on both the average reaction
94 rate and its deviation are used to infer a presumed distribution of knocking events around the mean knock
95 onset. An innovative definition for a probability of knocking cycles is proposed based on the same statistical
96 basis deriving from the model equations, differently from what previously proposed by Linse et al. [15]. An

97 initial application of the PDF-knock model was presented by the authors in [16], and the application on a
 98 knock-limited turbocharged GDI engine successfully predicted 6% of knocking cycles while the ensemble
 99 average realization was knock-safe. If a traditional RANS knock model was used, a knock-safe condition
 100 would have emerged, with no further information available on knock probability and lack of correlation with
 101 the experimental acquisitions. Conversely, the use of the presented PDF-knock model gave a quantitative
 102 information regarding the presumed fraction of knocking cycles affecting the mean simulation for a given
 103 operating condition, thus enhancing the meaning of a RANS simulation of knock with a typical test-bench
 104 acquisition dataset. This initial application motivated the development of the statistical knock model and the
 105 application on a research single-cylinder engine presented in this paper.

106 In the next section the details of the knock model are presented, which is based on detailed chemistry
 107 tabulation to accurately reproduce the local reaction rate. A statistically-based treatment accounting for
 108 presumed turbulence-chemistry interaction is presented and transport equations for the local perturbation of
 109 the thermal and mixing state are introduced. Finally, the derivation of the mean knock precursor and of its
 110 variance are presented. The model is applied to an optically accessible GDI engine, and the knock prediction
 111 given by the presented model is compared to the experimental outcomes in terms of frequency of knocking
 112 cycles. A criterion is also proposed to correlate the results from the Probability Density Function (PDF)
 113 based knock model with the number of knocking cycles, and the potentiality and the limitations of the
 114 presented model are critically presented and discussed.

115

116 **Presumed-PDF Knock Model**

117 *Cell-Average Reaction Rate*

118 The first step of the presented model is based on the calculation of a cell-wise average reaction rate. A
 119 procedure for the calculation of the autoignition (AI) delay is presented in [17, 18] and it is deputed to the
 120 interpolation of a cell-specific delay time from a pre-calculated database of calculated delay times $\tilde{\tau}$. Multi-
 121 dimensional interpolation is carried out considering the local Favre-averaged physical conditions, i.e. the
 122 input vector φ for the delay time interpolation considers the density-average values for each of absolute
 123 pressure, unburnt temperature, equivalence ratio and residuals mass fraction (Eq. 1).

$$124 \quad \varphi = \varphi(\tilde{p}, \tilde{T}_u, \tilde{\Phi}, \tilde{Y}_{EGR}) \quad (1)$$

125 The φ vector lists the independent variables that govern a multiple interpolation technique whose result is the
 126 AI delay time $\tilde{\tau}$. In this study the Andrae et al. [19] Toluene Reference Fuel (TRF) mechanism is adopted to
 127 generate a detailed look-up table of AI delays reproducing the autoignition behavior of a commercial RON95
 128 European gasoline, corresponding to the fuel quality used in the experiments. Once the local $\tilde{\tau}$ is known, it
 129 can be time-integrated in the Livengood and Wu [20] or in the Lafossas et al. [21] models.

130 The limitation of the crude use of the cell-wise average $\tilde{\tau}$ value to represent the local reaction rate is the
 131 concept that a perfectly uniform value of pressure, unburnt temperature, equivalence ratio and residuals mass
 132 fraction is assumed in the cell. As a consequence, every fluid cell is considered as a laminar well-stirred
 133 reactor. Even in a RANS framework, ensemble average turbulence may affect the local thermal and mixing
 134 states around the mean value which could, in turn, induce variations in the reactivity of the unburnt charge.
 135 Such an effect would be completely neglected by using a unique $\tilde{\tau}$ value. Therefore the model is extended to
 136 provide information regarding not only the average knock onset but also its dispersion around the mean
 137 value; details are presented in the next sections.

138 *PDF-Knock Model Equations*

139 Two additional transport equations are introduced to account for the statistical reconstruction of the physical
 140 states which may simultaneously be present in each fluid cell. Their dispersion around the mean value is

141 originated by the local turbulence intensity, ultimately leading to two independent knock precursors and to a
 142 statistically-based knock prediction. Dedicated transport equations are solved to account for local values of
 143 unburnt enthalpy and mixture fraction variance, $\widetilde{h_u^{n2}}$ and $\widetilde{Z^{n2}}$ respectively. They are reported in Eq. 2 and 3.

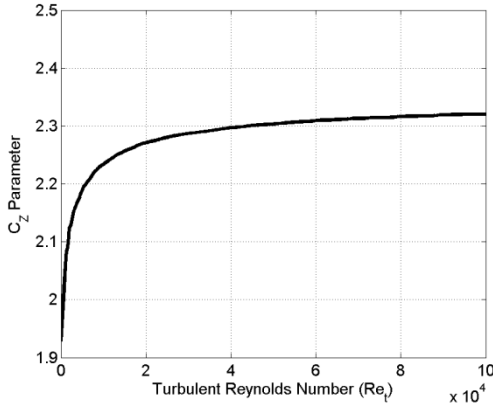
$$144 \quad \frac{\partial \bar{\rho} \widetilde{h_u^{n2}}}{\partial t} + \frac{\partial}{\partial x_j} \left[\bar{\rho} \widetilde{v}_j \widetilde{h_u^{n2}} - \left(\bar{\rho} D_{\widetilde{h_u^{n2}}} + \frac{\mu_t}{\sigma_t} \right) \frac{\partial \widetilde{h_u^{n2}}}{\partial x_j} \right] = 2 \frac{\mu_t}{\sigma_t} \left(\frac{\partial \widetilde{h_u}}{\partial x_j} \right)^2 - \frac{\bar{\rho}}{\tau_Z(Re_t)} \widetilde{h_u^{n2}} \quad (2)$$

$$145 \quad \frac{\partial \bar{\rho} \widetilde{Z^{n2}}}{\partial t} + \frac{\partial}{\partial x_j} \left[\bar{\rho} \widetilde{v}_j \widetilde{Z^{n2}} - \left(\bar{\rho} D_{\widetilde{Z^{n2}}} + \frac{\mu_t}{\sigma_t} \right) \frac{\partial \widetilde{Z^{n2}}}{\partial x_j} \right] = 2 \frac{\mu_t}{\sigma_t} \left(\frac{\partial \widetilde{Z}}{\partial x_j} \right)^2 - \frac{\bar{\rho}}{\tau_Z(Re_t)} \widetilde{Z^{n2}} \quad (3)$$

146 The difference from the standard transport equations used for Favre-average unburnt enthalpy $\widetilde{h_u}$ and
 147 mixture fraction \widetilde{Z} is condensed in the dissipation terms, $-\frac{\bar{\rho}}{\tau_Z(Re_t)} \widetilde{h_u^{n2}}$ and $-\frac{\bar{\rho}}{\tau_Z(Re_t)} \widetilde{Z^{n2}}$ respectively. They
 148 are a function of the turbulent Reynolds number Re_t , from which a turbulent relaxation time-scale $\tau_Z(Re_t)$ is
 149 expressed from local values using the approach proposed by Fox [22] and reprised by Subramanian et al.
 150 [23]. The relaxation time-scale $\tau_Z(Re_t)$ is calculated based on the two equation k- ϵ turbulence model and on
 151 a C_Z parameter, and it is calculated as in Eq. 4:

$$152 \quad \tau_Z(Re_t) = C_Z(Re_t)^{-1} \frac{k}{\epsilon} \quad (4)$$

153 The C_Z variable links the local flow turbulence to the variance dissipation rate. To this aim, it is expressed as
 154 a function of the local turbulent Reynolds number Re_t as proposed in [23] and illustrated in Figure 1. A
 155 moderate dependence on the local Re_t is visible in Figure 1, and a first order approximation of this
 156 formulation would be to consider $C_Z = 2.2$.



157
 158 Figure 1. Variance dissipation rate C_Z parameter as a function of the local turbulent Reynolds number Re_t .

159 For low turbulent conditions (i.e. low Re_t), a small value of the $C_Z(Re_t)$ parameter is calculated, resulting in
 160 a long turbulent relaxation time-scale $\tau_Z(Re_t)$ from Eq. 4. As a consequence, the variance destruction
 161 operated by turbulence-operated mixing in Eq. 2 and 3 is slow and a high probability to find in-cell far from
 162 average states is accounted for. The opposite is verified for highly turbulent conditions. The perturbation of
 163 the local fluid state is not arbitrarily imposed, but it is derived from transport equations originating from
 164 turbulence intensity itself, hence no artificial or user-imposed variation of flow variables is introduced.
 165 Equations 2 and 3 constitute the fundamentals of the statistical treatment of the presented knock model and
 166 their application will be described in the next sections.

167 Finally, despite the absence of explicit spray-related terms in Eq. 2 and 3, the fuel spray affects variance
 168 fields by promoting gradients in the mean field of both \widetilde{Z} and $\widetilde{h_u}$ due to fuel evaporation and evaporative
 169 cooling, respectively. This leads to variance production, as accounted for by the first term on the RHS of Eq.

170 2 and 3. Also, the spray-induced turbulence acts as a local thermo-mechanical mixer, which is considered by
 171 the dissipation terms on the RHS of Eq. 2 and 3.

172 *Statistical Description of In-Cell Reaction Rate*

173 Both mean values and their variances are considered for enthalpy h and mixture fraction Z . As for cell-
 174 averaged values, these are calculated from standard Favre-averaged Navier-Stokes transport equations,
 175 whereas local variance values are derived from the presented two additional transport equations (Eq. 2 and
 176 3).

177 As a first step, the mixture fraction Z is examined. Given the mean \bar{Z} and the variance \bar{Z}''^2 , a normal
 178 Gaussian distribution around the mean value in the mixture fraction space is assumed, whose spreading is
 179 represented by \bar{Z}''^2 . The probability $P(Z)$ to find the generic Z mixture quality in the cell volume is
 180 represented by Eq. 5.

$$181 \quad P(Z) = \frac{1}{\sqrt{\bar{Z}''^2} \sqrt{2\pi}} \cdot \exp\left[-\frac{(Z-\bar{Z})^2}{2 \cdot \bar{Z}''^2}\right] \quad (5)$$

182 If a single variable fluctuation was of interest, an analogous treatment could be carried out for enthalpy h .
 183 However, in this model both mixture fraction Z and unburnt enthalpy h_u are affected by turbulence, as
 184 expressed by the variance values $\bar{h}_u''^2$ and \bar{Z}''^2 . Their joint effect has to be accounted for in each single cell
 185 and it is evaluated using a multi-variate Gaussian distribution, reported in its general form in Eq. 6 and
 186 considering a correlation coefficient ρ_{Zh} whose meaning will be described later.

$$187 \quad P(Z, h_u) = \frac{1}{2\pi \cdot \sqrt{\bar{Z}''^2} \sqrt{\bar{h}_u''^2} \sqrt{1-\rho_{Zh}^2}} \cdot \exp\left\{-\frac{1}{2(1-\rho_{Zh}^2)} \cdot \left[\frac{(\bar{Z}-\langle\bar{Z}\rangle)^2}{\bar{Z}''^2} + \frac{(\bar{h}-\langle\bar{h}\rangle)^2}{\bar{h}_u''^2} - \frac{2\rho_{Zh}(\bar{Z}-\langle\bar{Z}\rangle)(\bar{h}-\langle\bar{h}\rangle)}{\sqrt{\bar{Z}''^2} \cdot \sqrt{\bar{h}_u''^2}} \right] \right\} \quad (6)$$

188 A simplification of Eq. 6 could be introduced by assuming mixture fraction Z and unburnt enthalpy h_u as
 189 uncorrelated variables, implying $\rho_{Zh} = 0$ and leading to the simplified form in Eq. 7. This approximation is
 190 only used at this initial stage to describe the multi-variate model for the cell as a function of the local
 191 turbulence level.

$$192 \quad P(Z, h_u) = \frac{1}{2\pi \cdot \sqrt{\bar{Z}''^2} \sqrt{\bar{h}_u''^2}} \cdot \exp\left\{-\frac{1}{2} \cdot \left[\frac{(\bar{Z}-\langle\bar{Z}\rangle)^2}{\bar{Z}''^2} + \frac{(\bar{h}-\langle\bar{h}\rangle)^2}{\bar{h}_u''^2} \right] \right\} \quad (7)$$

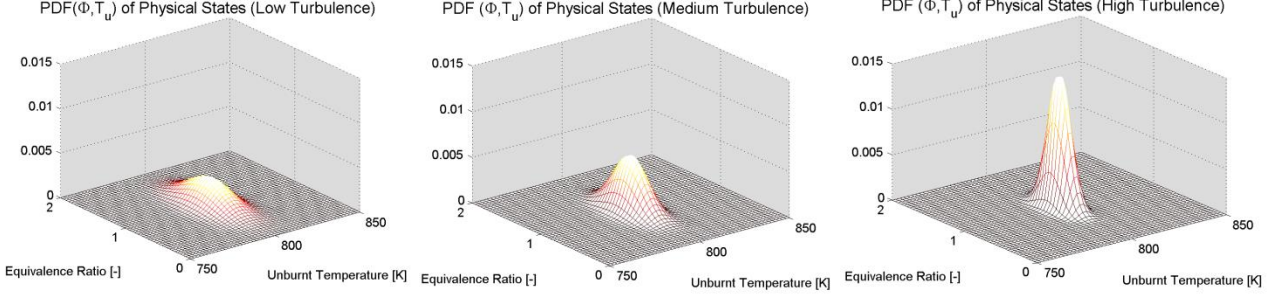
193 As a final step, the mixture fraction space is converted into an equivalence ratio one and the unburnt
 194 temperature T_u is substituted to enthalpy through Eq. 8 and 9.

$$195 \quad \bar{T}_u''^2 = \frac{\bar{h}_u''^2}{c_p} \quad (8)$$

$$196 \quad \bar{\Phi}''^2 = \alpha_{st} \cdot \frac{\bar{Z}''^2}{\bar{Y}_{O_2} + \bar{Y}_{N_2}} \quad (9)$$

197 In Eq. 8 c_p is the isobaric mixture specific heat, while in Eq. 9 α_{st} is the stoichiometric air-to-fuel ratio of
 198 the fuel-air mixture and \bar{Y}_{O_2} and \bar{Y}_{N_2} are the mass fractions of oxygen and nitrogen respectively. From a
 199 mathematical point of view, this treatment stands as a presumed statistical reconstruction of all the possible
 200 combinations of (Φ, T_u) which may exist in the cell and whose dispersion around the mean value is given by
 201 the local turbulent time scale. The expression reported in Eq. 7 represents the probability of a given (Φ, T_u)
 202 state to be present in the cell volume. The probability is maximum for the mean value pair $(\bar{\Phi}, \bar{T}_u)$, while it is
 203 progressively reduced for far-from-average states, although it is not null for these; this anticipates the
 204 limitation of a single AI delay to describe the whole cell reactor. The statistical two-dimensional model for

205 the fluid cell is graphically resumed in Figure 2 for different levels of turbulence, which is reflected by the
 206 amplitude of the multi-variate Gaussian model. The use of normal distribution for mixture fraction is
 207 motivated to keep the model assumptions to a minimum and to allow the use of a well-established multi-
 208 variate Gaussian distribution on Z and h_u . However, beta-distribution is another candidate choice for mixture
 209 fraction statistical representation, although it relevantly complicates the definition of a bi-variate distribution
 210 function such as the one in Eq. 6.



211

212 Figure 2. Multi-variate Gaussian-PDF distribution of physical states for the fluid cell in the presumed-PDF knock model. For the same
 213 most probable condition $(\bar{\Phi}, \bar{T}_u)$, increasing turbulence intensity levels (from left to right) lead to a more effective mixing and to a
 214 probability reduction for far from average states to exist.

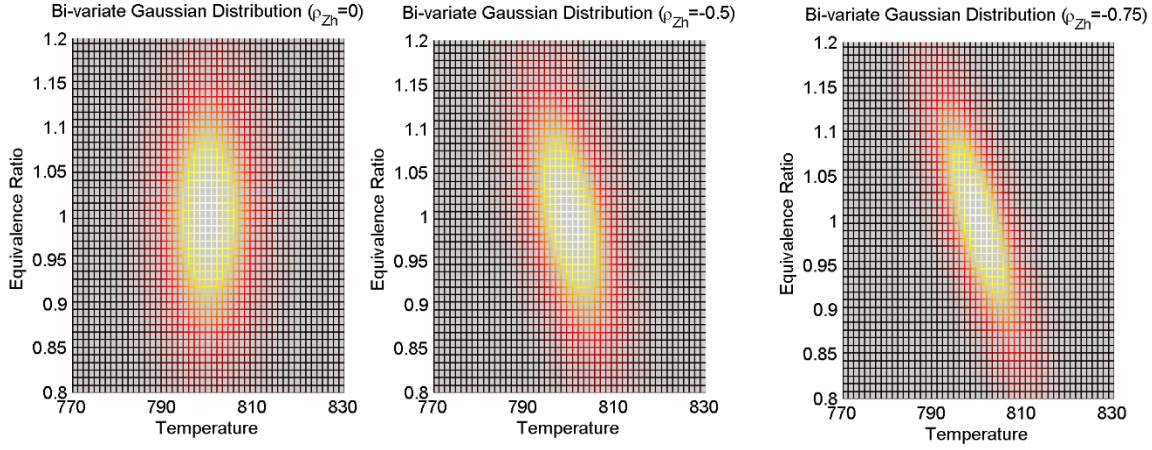
215 For the sake of numerical implementation, the multi-variate Gaussian distribution of physical conditions
 216 (Φ, T_u) is discretized in an arbitrary number of physical states. In the present study, a cell-wise discretization
 217 step of half a standard deviation is adopted for both equivalence ratio and temperature, i.e. it is based on the
 218 local values of $\sqrt{\bar{T}_u^2}/2$ and $\sqrt{\bar{\Phi}^2}/2$. Finally, a clipping distance from the mean value must be chosen in
 219 order to bound a finite in-cell physical space: in the present analysis a clipping is adopted at two standard
 220 deviations of each variable, i.e. $\pm 2 \cdot \sqrt{\bar{T}_u^2}$ and $\pm 2 \cdot \sqrt{\bar{\Phi}^2}$. A consequence of this is that approx. 95% of the
 221 overall probability of mixture states is accounted for. Each of the two independent variables is therefore
 222 divided into 9 discrete values and the distribution of the in-cell states counts 9^2 conditions. Sensitivity
 223 analyses showed that this is a balanced compromise between the resolution of the discretized distribution and
 224 the amplitude of the simulated states. The result of the outlined procedure is a discrete clipped multi-variate
 225 Gaussian distribution. Due to the discretization operation and the boundary truncation, a final re-
 226 normalization is carried out to re-normalize the sum of all the represented discrete states to unity.

227 The presence of the correlation coefficient ρ_{Zh} in Eq. 6 is used here to account the degree of relationship
 228 between unburnt temperature variation and mixture fraction. This is needed since this is a likely scenario in a
 229 modern GDI unit, where intense fuel stratification is observed. Charge non-homogeneity may persist until
 230 the end of the compression stroke, and it causes temperature inhomogeneity due to the dependency of the
 231 specific heat on mixture quality. The correlation coefficient ρ_{Zh} is calculated in the model at each iteration
 232 through the analysis of the in-cylinder instantaneous \tilde{Z} and \tilde{h}_u fields and it is modelled using a Pearson-like
 233 formulation as in Eq. 10:

$$234 \rho_{Zh} = \frac{\sigma_{Zh}}{\sigma_{\tilde{Z}} \cdot \sigma_{\tilde{h}_u}} = \frac{\sum_i [(\tilde{Z}_i - \langle \tilde{Z} \rangle) \cdot (\tilde{h}_{u,i} - \langle \tilde{h}_u \rangle)]}{\sqrt{\sum_i (\tilde{Z}_i - \langle \tilde{Z} \rangle)^2} \cdot \sqrt{\sum_i (\tilde{h}_{u,i} - \langle \tilde{h}_u \rangle)^2}} \quad (10)$$

235 In Eq. 10, the $\sigma_{\tilde{Z}}$ and $\sigma_{\tilde{h}_u}$ terms are the standard deviations of the mean Favre-average in-cylinder \tilde{Z} and \tilde{h}_u
 236 fields. Therefore, the ρ_{Zh} coefficient is dynamically calculated at each iteration based on the instantaneous
 237 modeled mean \tilde{Z} and \tilde{h}_u fields, from which the spatial average $\langle \tilde{Z} \rangle$ and $\langle \tilde{h}_u \rangle$ values are calculated. The ρ_{Zh}
 238 term is found to be always negative: high \tilde{Z} cell-values (i.e. rich-in-fuel regions) are more likely associated to
 239 low \tilde{h}_u . This is a consequence of the relationship between \tilde{Z} and \tilde{h}_u deriving from the mixture isobaric
 240 specific heat. The instantaneous local ρ_{Zh} correlation coefficient modifies the bi-variate Gaussian model for

241 the in-cell conditions as illustrated in Figure 2 for several ρ_{Zh} parameter values. In Figure 3 the equivalence
 242 ratio is used instead of \tilde{Z} to represent fuel concentration. Hotter states are associated with leaner mixtures
 243 (bottom-right side in Figure 3) and the same is for cooler and richer conditions (upper-left side in Figure 3),
 244 while hot and rich (upper-right) or cool and lean (lower-left) combinations are less probable.



245

246 Figure 3. Bi-variate Gaussian distribution for the in-cell statistical states as a function of the ρ_{ZT} correlation coefficient: $\rho_{Zh} = 0$
 247 (left, uncorrelated equivalence ratio and \tilde{h}_u), $\rho_{Zh} = -0.5$ and $\rho_{Zh} = -0.75$ (middle and right, negatively correlated equivalence ratio
 248 and \tilde{h}_u).

249

250 **Knock Precursor Variance**

251 From a general point of view, once a global reaction rate $\tilde{\omega} = \tilde{\tau}^{-1}$ is known a knock precursor growth rate
 252 can be calculated in the same way as the Livengood and Wu knock integral function \tilde{I} . This can be
 253 transported as a generic scalar with an equation as Eq. 11.

$$254 \quad \frac{\partial \tilde{\rho} \tilde{I}}{\partial t} + \frac{\partial}{\partial x_j} \left[\tilde{\rho} \tilde{v}_j \tilde{I} - \left(\tilde{\rho} D_{\tilde{I}} + \frac{\mu_t}{\sigma_t} \right) \frac{\partial \tilde{I}}{\partial x_j} \right] = \tilde{\rho} \tilde{\omega} \quad (11)$$

255 The difference introduced by the presumed-PDF treatment lies in the definition of the $\tilde{\omega}$ term. Since a variety
 256 of physical states is statistically possible in the single fluid cell, a distribution of reaction rates is also to be
 257 considered in the cell volume. The theoretical global reaction rate follows a more complex definition and it is
 258 expressed as in Eq. 12.

$$259 \quad \tilde{\omega} = \int_V P(\Phi, T) \cdot \omega(\Phi, T) dV = \int_V P(\Phi, T) \cdot \frac{1}{\tau(\Phi, T)} dV \quad (12)$$

260 The calculation of the integral can be numerically challenging since an analytical function of $\tilde{\omega}(\Phi, T)$ is not
 261 known a priori, hence an assumption is made considering the dispersion of the in-cell reaction rates as the
 262 sum of a mean term and a contribution due to fluctuations. This last can be either positive or negative, i.e. it
 263 can accelerate or slow down the global reaction rate depending on the considered local physical state. Since
 264 the focus of this study is on the earliest probability that a portion of a fluid cell experiences autoignition, just
 265 the faster than average part of the reaction rate distribution is of interest.

266 These arguments lead to the representation of the knock inceptor reaction rate $\omega_{PDF,peak}$ by means of an
 267 average value $\omega_{PDF,aver}$ and an accelerating contribution given by its root mean square (rms) ω_{rms} value
 268 (Eq. 13).

$$269 \quad \omega_{PDF,peak} = \omega_{PDF,aver} + \omega_{rms} \quad (13)$$

270 The first term on the right side is obtained by a PDF-weighted averaging operation of the population of
 271 reaction rates calculated based on the discrete multi-variate PDF space, hence the $\omega_{PDF,aver}$ name (Eq. 14).

$$272 \quad \omega_{PDF,aver} = \sum_{i=1}^{\Phi_{tot}} \sum_{j=1}^{T_{tot}} P(\Phi_i, T_j) \cdot \frac{1}{\tau(\Phi_i, T_j)} d\Phi dT \quad (14)$$

273 The second term is calculated as the difference between the $\omega_{PDF,aver}$ term and the faster than average
 274 reacting state considered in the discrete cell representation. It represents the root mean square of the faster
 275 than average reaction rates within the fluid cell. Following an analogous $\pm 2 \cdot \sqrt{\tau^{n2}}$ clipping for AI delays,
 276 this reads as Eq. 15 and corresponds to the reaction rate of the 2.5% of the fastest-reacting portion.

$$277 \quad \omega_{+2\sigma} = \frac{1}{\tau} \Big|_{-2\sigma} \quad (15)$$

278 Finally, the ω_{rms} term is calculated as in Eq. 16 and it represents the net increase in reaction rate due to the
 279 accelerating contribution of the statistically present faster than average states.

$$280 \quad \omega_{rms} = \frac{\tau|_{PDF,aver} - \tau|_{-2\sigma}}{\tau|_{PDF,aver} \cdot \tau|_{-2\sigma}} \quad (16)$$

281 Once all the needed terms are available, the time integration of a knock integral function can be calculated
 282 considering Eq. 13, and it is manipulated as in Eq. 17 to split the integration of the mean reaction rate and its
 283 statistically faster reacting portion:

$$284 \quad \tilde{I} = \int_{t_0}^t \tilde{\omega} dt = \int_{t_0}^t \omega_{PDF,aver} dt + \int_{t_0}^t \omega_{rms} dt \quad (17)$$

285 The decomposition in Eq. 17 immediately leads to the independent calculation of two knock precursors,
 286 $\tilde{I}_{PDF,aver}$ and \tilde{I}_{rms} respectively (Eq. 18). The former expresses the average chemical reaction rate towards
 287 autoignition, while the latter is the precursor variance contribution given by the turbulence intensity.

$$288 \quad \tilde{I}_{PDF,peak} = \tilde{I}_{PDF,aver} + \tilde{I}_{rms} \quad (18)$$

289 The average knock precursor and its variance are modelled through dedicated transport equations, Eq. 19 and
 290 20 respectively.

$$291 \quad \frac{\partial \bar{\rho} \tilde{I}_{PDF,aver}}{\partial t} + \frac{\partial}{\partial x_j} \left[\bar{\rho} \tilde{v}_j \tilde{I}_{PDF,aver} - \left(\bar{\rho} D_{\tilde{I}_{PDF,aver}} + \frac{\mu_t}{\sigma_t} \right) \frac{\partial \tilde{I}_{PDF,aver}}{\partial x_j} \right] = \bar{\rho} \omega_{PDF,aver} \quad (19)$$

$$292 \quad \frac{\partial \bar{\rho} \tilde{I}_{rms}}{\partial t} + \frac{\partial}{\partial x_j} \left[\bar{\rho} \tilde{v}_j \tilde{I}_{rms} - \left(\bar{\rho} D_{\tilde{I}_{rms}} + \frac{\mu_t}{\sigma_t} \right) \frac{\partial \tilde{I}_{rms}}{\partial x_j} \right] = \bar{\rho} \omega_{rms} \quad (20)$$

293 Since the model aim is to track an autoignition probability for the fluid cell, the heat release due to potential
 294 knock is purposely not simulated. If autoignition heat was simulated, when AI is met for a portion of the cell
 295 due to faster than average states it would affect all the other realizations (e.g. the average knock onset) by
 296 varying the local thermo-physical conditions, while it is more interesting to transport both average and
 297 maximum probability states within the Gaussian-based model and independently track their time-history.

298

299 **Experimental Apparatus and Engine Knock Characterization**

300 Measurements were performed on a single-cylinder optically accessible DISI engine; whose main
 301 specifications are carefully detailed in [24] and here briefly resumed for the sake of completeness in Table 1

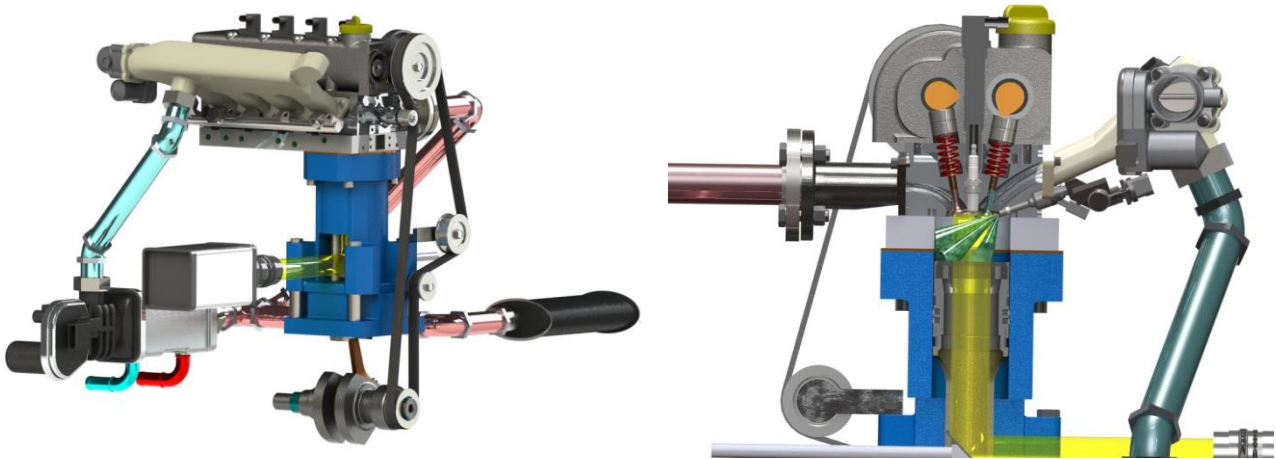
302 along with the operating conditions. The crank angle reference is made to the TDC at the end of
303 compression.

Displacement	$\approx 399 \text{ cm}^3$
Bore	79.0 mm
Stroke	81.3 mm
Connecting Rod	143 mm
Compression Ratio	10:1
Injection pressure	100 bar
Engine Speed	$\approx 2000 \text{ rpm}$
Boost pressure	0.5 bar
Spark Advance	15 CA bTDC

304 Table 1. Single cylinder optically accessible SI engine characteristics.

305 The engine is equipped with the cylinder head of a 1.4 litre currently made SI turbocharged power unit. The
306 wall-guided fuel injection system features a side-mounted injector with a six-hole configuration and the
307 spark plug is centrally located, as reported in Figure 4. Optical access is ensured through an 18 mm-thick
308 fused silica window fixed on the piston crown featuring a Bowditch design [25] with a 45 degree UV-
309 enhanced mirror. Self-lubricating piston rings ensured oil-free operation, thus avoiding contamination of the
310 visible field of view. More details into the application of optical techniques on this engine and other specific
311 challenges are available in [26, 27]. Coolant and lubricant temperature were monitored and maintained at
312 330 K using a thermal conditioning unit. Engine speed was set at 2000 rpm, while start of injection was
313 triggered at 300 CA bTDC with a single-pulse strategy at a pressure equal to 100 bar. The overall air-to-fuel
314 ratio was set close to stoichiometry ($\lambda \approx 1.05$) and monitored using an oxygen sensor on the exhaust line, with
315 an accuracy of $\pm 1\%$.

316

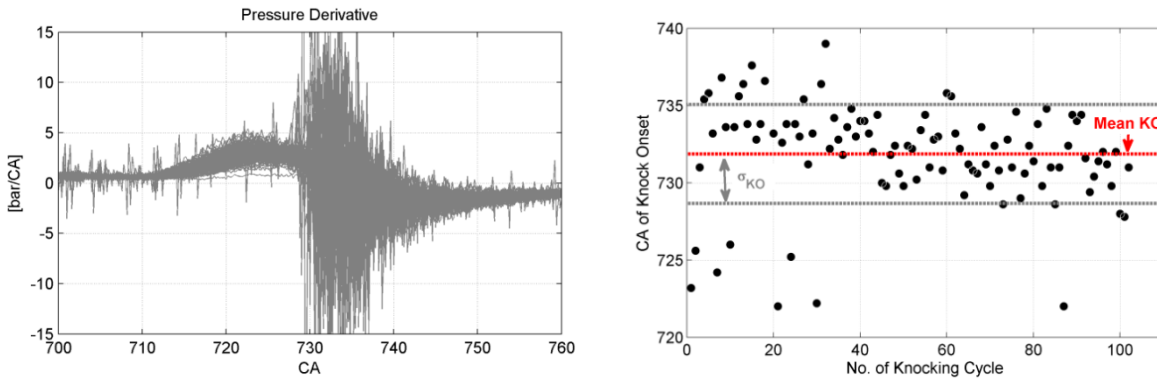


317

318 Figure 4. Experimental apparatus for the optically accessible SI engine.

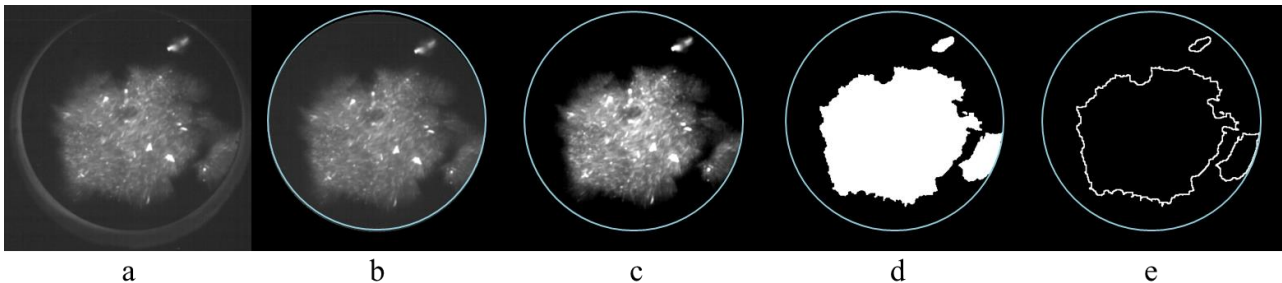
319 A turbocharged operating condition was examined in this study, with 0.5 bar boost pressure and intake
320 manifold temperature around 315 K. Spark timing was set at 15 CA bTDC, and this also constituted the
321 trigger for recording the optical measurements. The adoption of an instrumented GDI turbocharged unit
322 represents an optimal testing for the presented knock model, allowing to include in the analysis the effects of
323 stratified mixture distribution and high end-gas thermal loading common to most of the modern SI
324 production units. A dataset of in-cylinder pressure measured (with a resolution of 0.2 CA) during 173
325 consecutive firing cycles were recorded through a piezo-electric transducer (that featured an accuracy of
326 $\pm 1\%$) flush-mounted on one side of the combustion chamber between an intake and an exhaust valve. The
327 experiments were carried out using a commercial RON95 gasoline, and a knock-affected condition is

328 observed from the cycle-resolved in-cylinder pressure derivative reported in Figure 5 (left). An arbitrary
 329 limit of pressure derivative was chosen equal to 5 bar/CA to discern between knocking and non-knocking
 330 cycles. The result of this filtering is that 109 out of 173 cycles exceed this criterion, depicting a 63% fraction
 331 of experimentally knocking cycles for this operation. The CA of knock onset for this subset of cycles is
 332 reported in Figure 5 (right), and the mean CA for knock onset for this portion of cycles is +11.9 CA aTDC,
 333 with a standard deviation equal to 3.2 CA. This illustrates the ‘run-away’ behavior of knock, with the
 334 specific pressure oscillations being more evident for cycles at the end of the recorded dataset.



335
 336 Figure 5. Cycle-resolved in-cylinder pressure derivative (left) and CA of knock onset for the subset of knocking cycles (right).

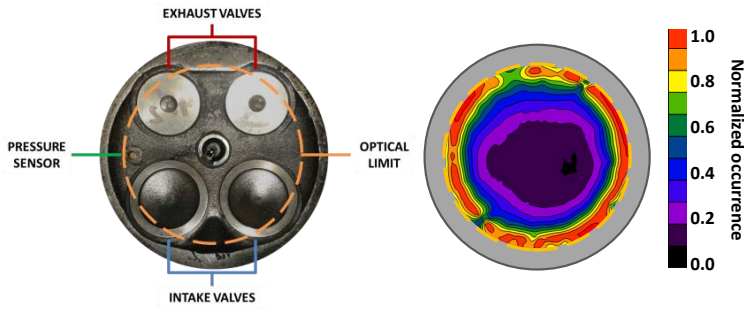
337 Cycle resolved visualization was performed for 100 consecutive cycles out of the 173 via a CMOS camera
 338 (Optronis CamRecord 5000 – 512 x 512 pixel, 8-bit pixel digitization and 5000 frame per second at full chip)
 339 equipped with a 50 mm focal Nikon lens. The exposure time was fixed at 166.7 μ s and the dwell time
 340 between two consecutives images was 200 μ s (2.4 CAD at 2000 rev/min). A custom designed image
 341 processing using Vision Assistant of National Instruments allowed to retrieve quantitative information from
 342 the combustion visualizations even for images with low signal to noise ratio. As sketched in Fig. 6 (a-e),
 343 after the application of an appropriate circular mask (a->b) to cut the spurious light from reflections at the
 344 boundaries of the optical window of the piston crown, a look-up table (LUT) transformation [28] was used to
 345 adjust the brightness at 174, contrast at 73 and the gamma value at 0.76 (b->c). Then, thresholding was
 346 performed by fixing the minimum image intensity at 21 on 256 grey-scales (Fig. c->d). Thus, images were
 347 segmented into two regions, foreground and background respectively, obtaining a binarized image [29].
 348 Finally, the contours of flames were defined (d->e) and the related coordinates in pixels were stored. In order
 349 to perform a frequency map of autoignition events, only the border coordinates of the flames in the end-gas
 350 detected at fixed delay from the spark timing were considered. It should be noted that the difference between
 351 the optical window and the engine bore determined a 5.25 mm thick blind circular crown; therefore, only
 352 autoignition flames sufficiently large to cover the distance between the wall and the optical crown limit can
 353 be considered for the evaluation of autoignition maps.



354
 355 Figure 6. Sketch of the image processing steps.

356 The experimentally measured knock probability is reported in Figure 7 through a spatial map of the
 357 normalized autoignition occurrence. The probability for the end-gases to undergo autoignition is assessed by
 358 means of the optical analysis carried out through the transparent piston window which allowed to identify the

359 distribution of the end-gas regions subjected to knock; the peak probability was found on the exhaust side
360 (top part in the picture), although knock is also probable on the intake side (low side in the picture).

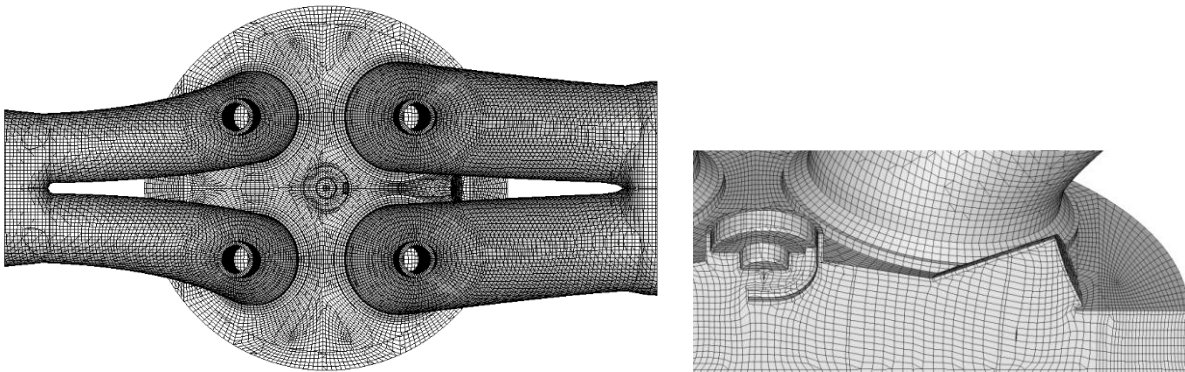


361

362 Figure 7. Map of normalized autoignition location (left) and CA of knock onset for the subset of knocking cycles (right).

363 3D CFD simulations

364 The 3D CFD analyses presented in this paper are carried out by means of a customized version of STAR-CD
365 v4.22. Time varying pressure boundary conditions derive from the experiments and they are used to validate
366 a 1D model of the engine, from which the corresponding temperature trace is extracted. Turbulence is
367 modelled though the $k-\epsilon$ RNG turbulence model for compressible flows. The grid adopted for the simulations
368 is reported in Figure 8 and it reproduces the whole combustion chamber and both the intake and exhaust
369 ports. A close-up of the spark plug geometry and of the injector region are presented in Figure 8 as well. The
370 total number of cells is approx. 1.48 M and 430000 at BDC and TDC respectively, while the average cell-
371 size is about 0.55 mm throughout the simulation.



372

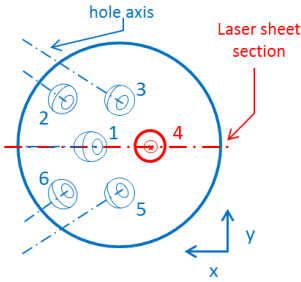
373 Figure 8. Computational grid (top) and spark plug and injector region detail (bottom).

374 Combustion is modelled with the Flame Surface Density (FSD) ECFM-3Z model [30], coupled with a
375 relatively simple algebraic ignition model based on a flame profile deposition to account for flame kernel
376 formation [31]. The fuel injector is a 6-hole full-cone GDI one whose nominal data are reported in Table 2
377 and whose nozzle orientation is sketched in Figure 9. The multi-hole liquid spray is modelled using a
378 Lagrangian approach, where the fuel atomization is replaced by a Rosin-Rammler droplet distribution
379 function. Nozzle-specific mass flow rate is prescribed as to reproduce experimental flow unbalance between
380 the nozzles. The effective nozzle diameter is evaluated using the Kuensberg 1D model [32]. The secondary
381 break-up is modelled by the Reitz and Diwakar approach [33]. Finally, spray is validated against experiments
382 carried out in a spray bomb at an injection pressure of 100 bar; the spray morphology and the penetration
383 curve are reported in Figure 10 at two instants after Start Of Injection (SOI), 400 ms and 800 ms
384 respectively. In Figure 10 the penetration curve of the simulated spray is also reported and it confirms the
385 satisfactory agreement with the experiments.

386 Finally, knock is modelled by means of the presented presumed-PDF knock model, which is coupled with
 387 the STAR-CD solver through in-house developed user-coding.

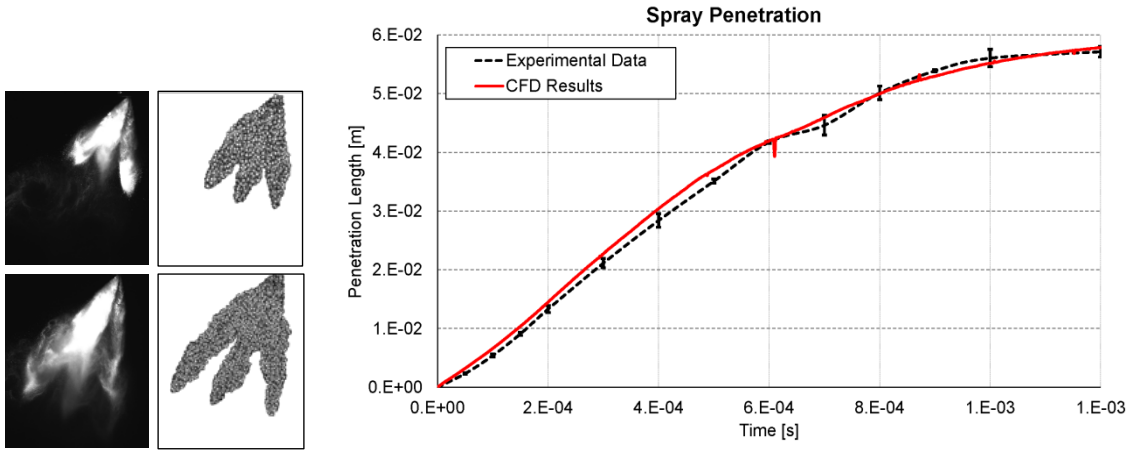
Nominal nozzle diameter	0.14 mm
Nominal nozzle length	0.196 mm
Number of nozzles	6

388 Table 2. Nominal injector data.



389

390 Figure 9. Sketch of the nozzle holes position and orientation.



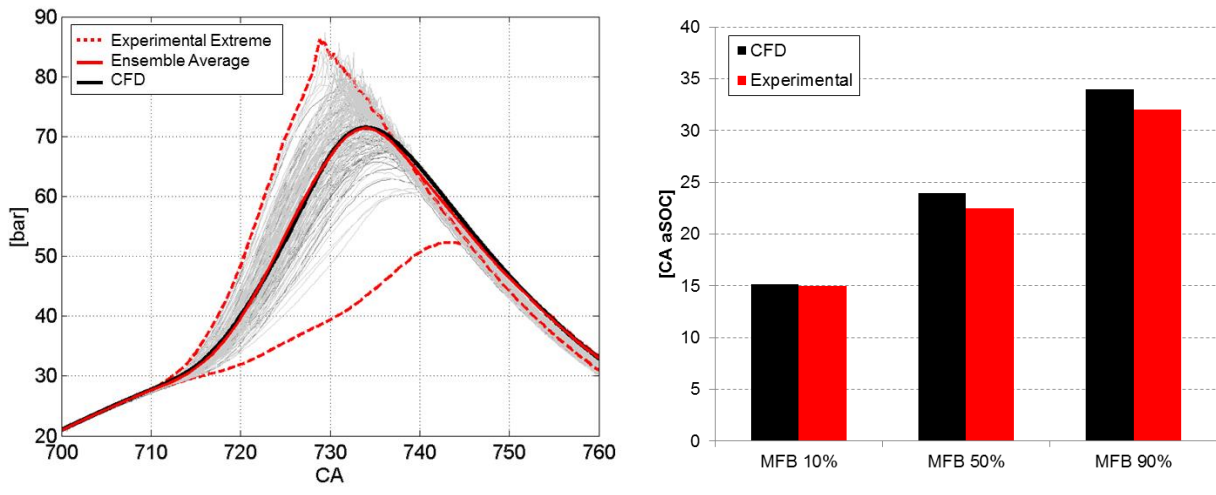
391

392 Figure 10. Simulated spray shape against experiments (left side) at 400 ms (top row) and 800 ms (bottom row) after SOI; comparison
 393 between experimental and simulated penetration curve (right side).

394

395 Results

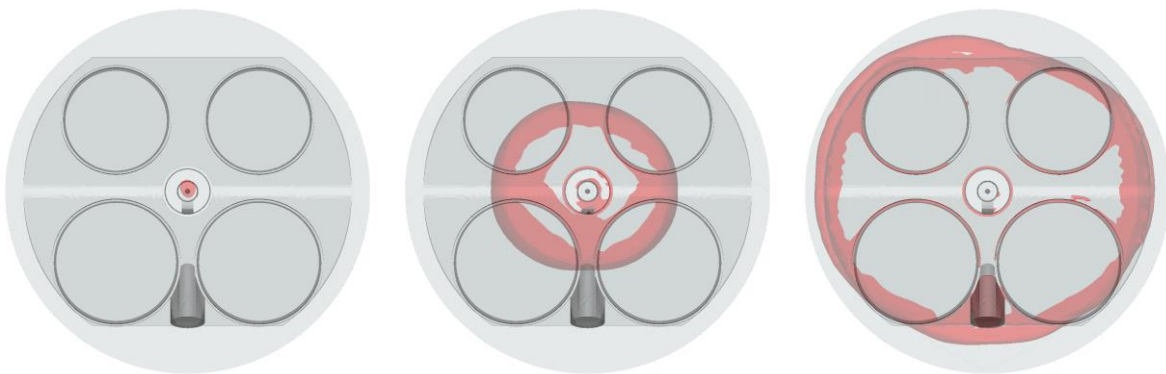
396 The set of pressure traces from each individual cycle, measured with 1% accuracy and 0.2 CA resolution, is
 397 reported in Figure 11, alongside with the calculated ensemble average trace and the extreme measured
 398 cycles. The combustion pressure trace from simulation is also reported in Figure 11 and the agreement
 399 between the CFD result and the ensemble average pressure trace assesses the validity of the simulation to
 400 represent the mean flame development behaviour. This is further confirmed by the agreement of the
 401 combustion indicators for 10%, 50% and 90% of fuel burnt.



402
403
404
405
406

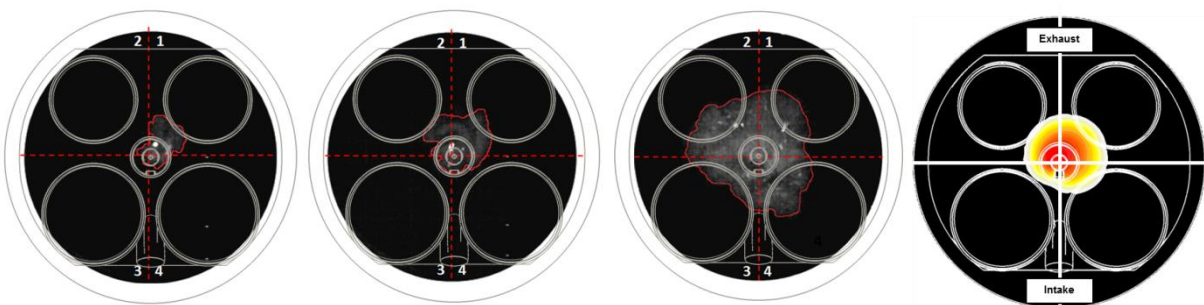
Figure 11. Left: CFD pressure trace (black solid line) compared with the experimental extreme cycles (red dashed lines) and ensemble average pressure traces (red solid line). Right: comparison of the main combustion phasing indicators for CFD and ensemble average of experimental cycles.

407 The mean propagating flame front is depicted in Figure 12 by the isosurface of the Favre-averaged
 408 combustion progress variable \tilde{c} at $\tilde{c} = 0.5$ value. Flame initiation is compared to the experimental imaging to
 409 analyze the simulation accuracy in representing the flame kernel evolution. Figure 13 shows that a flame
 410 kernel development towards the exhaust side of the combustion chamber (top side) is recurrently observed
 411 for three selected cycles at +9 CA aSOC, representative of a slow, an average and a fast burning cycles
 412 (cycle no. 31, no.75 and no.109, respectively). Despite the relatively simple flame deposition model for spark
 413 ignition, numerical simulation confirms this tendency by means of combustion progress variable \tilde{c} field and
 414 explains this behavior as due to mean flow convection of the reaction zone given by the residual tumble
 415 motion.



416

417 Figure 12. Isosurface of the Favre-averaged combustion progress variable $\tilde{c} = 0.5$ at -10 CA aTDC (left), TDC (middle) and +10
 418 CA aTDC (right).



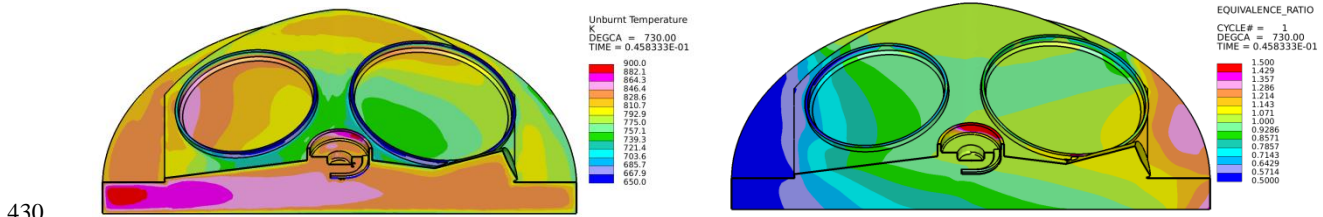
419

420 Figure 13. Flame contour for three selected cycles (cycle no. 31, no.75 and no.109, from left to right) at +9 CA aSOC (left side);
 421 combustion progress variable \tilde{c} field (rightmost figure).

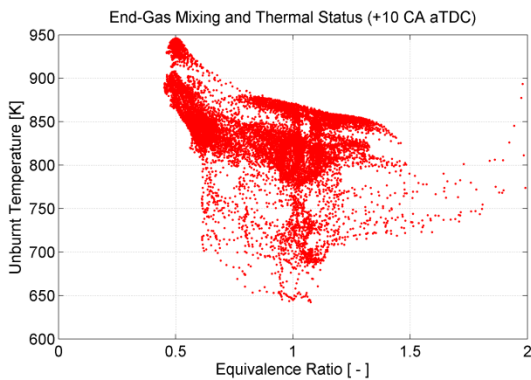
422

423 *Knock Prediction Simulation*

424 The presented knock model is applied to the simulated mean realization of combustion. In Figure 14 the
 425 unburnt temperature and the equivalence ratio field are represented at +10 CA aTDC. A detailed analysis of
 426 the end-gas condition is carried out for this CA. End-gases are identified through a conditioning on the
 427 Favre-average reaction progress variable \tilde{c} , by filtering cells whose \tilde{c} value is below 0.8. Figure 15 shows a
 428 scatter plot of the mixture composition against unburnt temperature, highlighting the promoted heating of the
 429 lean portion of peripheral mixture visible in Figure 14.

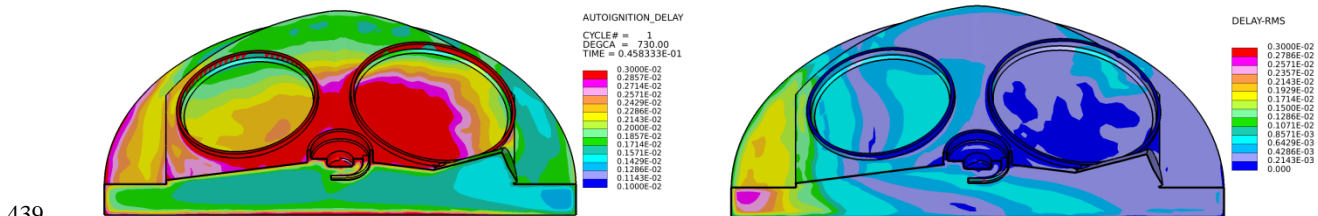


430
 431 Figure 14. Unburnt temperature (left side) and equivalence ratio field (right side) at +10 CA aTDC.



432
 433 Figure 15. Scatter plot of equivalence ratio against unburnt temperature for the end-gas region at +10 CA aTDC.

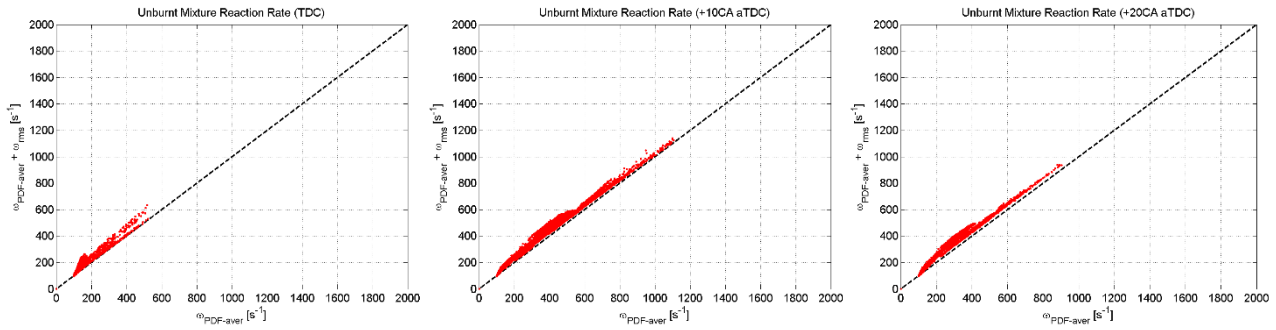
434 The field of average AI delay times and of its root mean square are reported in Figure 16. While the former
 435 field (left side), related to the gas phase average reaction rate (expressed as the inverse of the local AI delay
 436 time), shows local minima at the periphery of the intake valve and around the injector cavity, the latter (right
 437 side) visually suggests that local turbulence induces a more relevant degree of reactivity fluctuation on the
 438 exhaust side of the combustion chamber.



439
 440 Figure 16. Average AI delay time field (left side) and delay root mean square field (right side) at +10 CA aTDC.

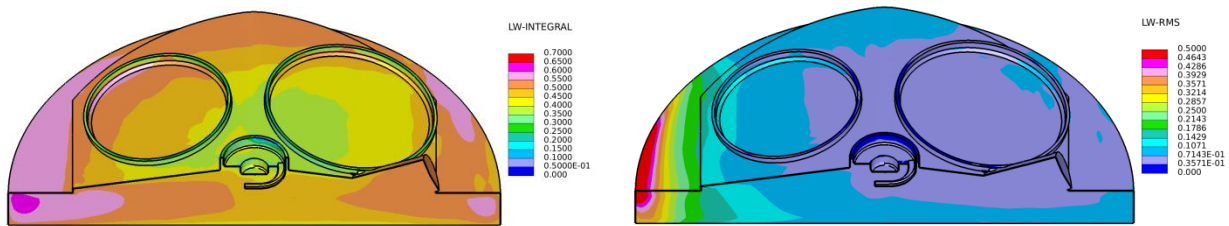
441 The peak reaction rate and its average counterpart are illustrated in the scatter plots in Figure 17 for the end-
 442 gas region at TDC, +10 CA aTDC and +20 CA aTDC. It is interesting to observe that the promotion of
 443 autoignition tendency given by the faster than average reacting states is present at all combustion stages, as

444 stated by the population of fluid cells clearly lying above the 45-degree line. This is verified for relatively low
 445 reaction rates (e.g. at TDC) as well as for highly reacting conditions (e.g. +10 CA aTDC).



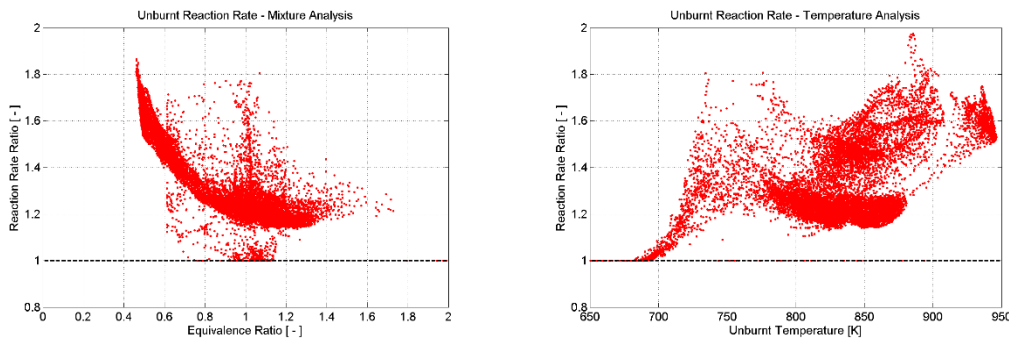
446
 447 Figure 17. Scatter plots of average reaction rate $\omega_{PDF,aver}$ (Eq. 14) against peak reaction rate $\omega_{PDF,peak}$ (Eq. 13) for the end-gas
 448 region: TDC (left), +10 CA aTDC (middle), +20 CA aTDC (right).

449 The field of the average knock precursor $\tilde{I}_{PDF,aver}$ and of its root mean square \tilde{I}_{rms} , as calculated by Eq. 19
 450 and 20, are represented in Figure 18. The average knock precursor field shows an evenly distributed
 451 population at both the exhaust and the intake sides, although the exhaust side of the combustion chamber
 452 (left side in figures) appears slightly more prone to knock. This is confirmed by the experiments, where
 453 knock onset locations were measured on both sides of the optical access. Furthermore, a $\tilde{I}_{PDF,aver}$ value
 454 below unity allows to consider the whole chamber as knock safe from an average point of view at such crank
 455 angle. Nonetheless, the magnitude of the precursor \tilde{I}_{rms} field is relevant compared to the mean value. In
 456 particular, its additional contribution on the exhaust side points out that turbulence-induced perturbations of
 457 the reaction rate lead to more probable knock in that region of the combustion chamber, despite the average
 458 realization is not knocking at +10 CA aTDC.



459
 460 Figure 18. Average knock precursor $\tilde{I}_{PDF,aver}$ field (left side) and precursor root mean square field \tilde{I}_{rms} (right side) at +10 CA
 461 aTDC.

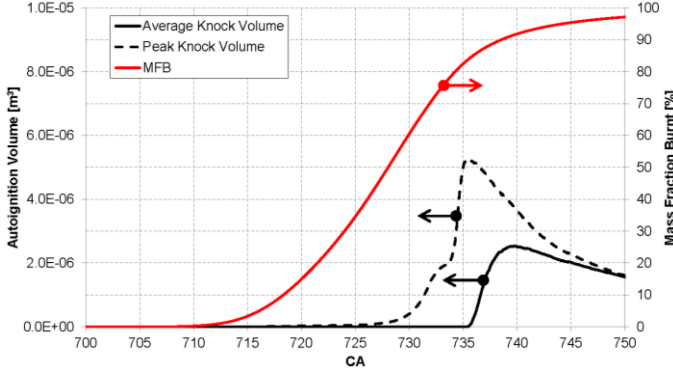
462 The degree of statistical knock tendency of the end-gases is further analyzed through the ratio of peak over
 463 average reaction rates as a function of the Favre-averaged fields of unburnt temperature and of the
 464 equivalence ratio, illustrated in Figure 19. Such analysis clearly shows that the leanest and hottest portion of
 465 the end gases, located on the exhaust side of the cylinder, are also those more subject to turbulence-induced
 466 reaction rate increase. This is accounted for by the ρ_{Zh} correlation coefficient calculated as in Eq. 10. This
 467 confirms the experimental evidence indicating the exhaust-side region as a knock critical area.



468
 15

469 Figure 19. Scatter plot of the ratio of peak over average reaction rate for the unburnt mixture at +10 CA aTDC as a function of the
 470 unburnt temperature (left) and of the equivalence ratio (right).

471 Finally, the volume of the end-gas region where the autoignition criterion is met for both the average knock
 472 precursor $\tilde{I}_{PDF,aver}$ and the peak precursor $\tilde{I}_{PDF,peak}$ is illustrated in Figure 10 together with the simulated
 473 mass fraction burnt (MFB) curve.



474
 475 Figure 20. Autoignition volume as predicted by the average $\tilde{I}_{PDF,aver}$ and the peak $\tilde{I}_{PDF,peak}$ knock precursors (black lines), together
 476 with the ensemble average MFB curve (red line).

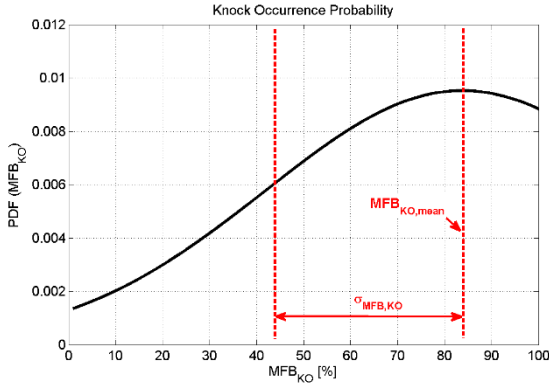
477

478 Definition of Knock Probability in RANS

479 The knock prediction given by the presented model is analysed to reconstruct a fraction of knocking cycles
 480 to be compared with the experimental evidence. Knock occurrence is observed through the mass fraction of
 481 fuel which is burnt at knock onset (hereafter MFB_{KO}). If the cell-average $\tilde{\tau}$ value alone was used, the only
 482 information available from the analysed engine would be that the ensemble average cycle is knocking after
 483 +15CA aTDC, but no conclusions could be inferred regarding the dispersion around this value.

484 The additional information given by the presented presumed-PDF model is the estimation of a probability
 485 function around the mean value, which is obtained from the knock occurrence of the peak knock precursor
 486 $\tilde{I}_{PDF,peak}$. This is used to define a second knock phasing indicator, i.e. $MFB_{KO,peak}$. Given the stochastic
 487 occurrence of knock, it is reasonable to assume a normal Gaussian distribution for knock occurrence, which
 488 is centred in $MFB_{KO,mean}$ with a standard deviation $\sigma_{MFB_{KO}}$ derived from $MFB_{KO,peak}$. In the considered
 489 case, $MFB_{KO,mean}$ is equal to 83.8% while $\sigma_{MFB_{KO}}$ is 39.8%. These values are based on a minimum non-null
 490 value of autoigniting volumes in the end-gas imposed as 1 mm^3 needed to avoid the spurious autoignition of
 491 individual cells to be considered. Based on these indicators a probability function of MFB_{KO} is reconstructed
 492 following Eq. 21 and it is illustrated in Figure 21.

$$493 \quad P(MFB_{KO}) = \frac{1}{\sigma_{MFB_{KO}} \sqrt{2\pi}} \cdot \exp \left[-\frac{(MFB_{KO} - MFB_{KO,mean})^2}{2 \cdot \sigma_{MFB_{KO}}^2} \right] \quad (21)$$



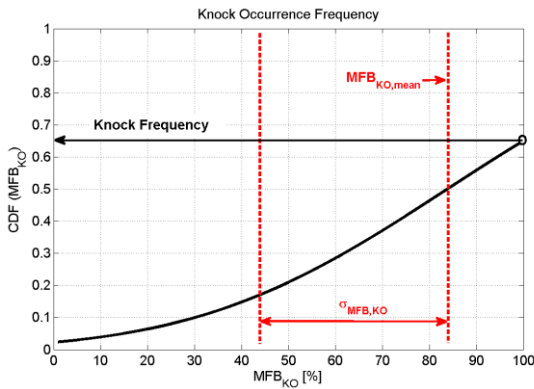
494

495 Figure 21. Assumed Gaussian-PDF of the percentage of burnt fuel at knock onset MFB_{KO} .

496 Given the above reconstruction for knock occurrence distribution, it is possible to calculate the cumulative
 497 probability of cycles exhibiting knock before the completion of regular combustion, i.e. 100% of burnt fuel.
 498 This is calculated as the Cumulative Distribution Function (CDF) of the above distribution, which is reported
 499 calculated in Eq. 22 and illustrated in Figure 22.

$$500 \quad CDF(MFB_{KO}) = \frac{1}{2} \cdot \left[1 + erf \left(\frac{MFB_{KO} - MFB_{KO,mean}}{\sqrt{2} \cdot \sigma_{MFB_{KO}}} \right) \right] \quad (22)$$

501



502

503 Figure 22. Cumulative Distribution Function of the percentage of burnt fuel at knock onset MFB_{KO} .

504 Since the region of interest is limited to the probability to have a knocking cycle before the regular
 505 combustion finalization, the cumulative probability to verify this condition is given by Eq. 22 calculated at
 506 the limit value, i.e. $CDF(MFB_{KO})|_{MFB_{KO}=100\%}$. In this case the knock frequency value is 65.8%, stating that
 507 approximately 66% of the possible realizations reach the conditions for autoignition in a portion of their
 508 volume, while the remaining 34% is knock-safe. This result is in very good agreement with the experimental
 509 evidence showing that a fraction of 63% of the measured cycles is knocking. This information is inferred
 510 from a single RANS simulation, while the average knock prediction alone would be unable to estimate any
 511 knock dispersion around the mean value.

512 It is important to underline that the aim of the presented model is neither to substitute a multiple cycle LES
 513 simulation, which remains the only way to properly simulate most of the CCV-promoting processes, nor to
 514 identify the exact fraction of knocking cycles measured during the experiments. The presented presumed-
 515 PDF model is a numerical tool to identify the regions of the combustion chamber which are statistically more
 516 prone to autoignition, and this information is inferred by a combination of an average knock precursor and a
 517 statistical description of the reaction rate deviation produced by local gradients and dissipated by local
 518 turbulent intensity. Since RANS simulations are the most appropriate tool to investigate the mean behaviour

519 of a fluid system (e.g. a new engine concept), the indications from the presumed-PDF model may provide
520 useful statistical information on the probability to trigger potentially damaging knocking events.

521 **Conclusions**

522 In this paper a statistics-based knock model is presented in the context of RANS combustion simulation,
523 which couples RANS traditional equations with the transport of variances for the physical conditions
524 affecting local reaction rate. The model is based on separate transport equations for both the mixing and the
525 thermal variance originated by local mean gradients and turbulent scales. They are combined to reconstruct a
526 statistical model for the in-cell reaction rate, which is represented though a clipped multi-variate Gaussian
527 distribution of probability. Two independent knock precursors are transported, in order to account for both
528 the ensemble average knock proximity and its variance around the mean value. The combined use of the
529 precursors is able to outline a statistically-based description of the in-cell reaction rate distribution.

530 When applied to a laboratory GDI engine with optical access, the results from the presumed-PDF knock
531 model assesses knock onset on the exhaust side of the combustion chamber. This is the area where flame
532 visualization indicated the highest knock probability, and numerical simulations showed that this region
533 suffers of lean and hot end-gases, promoting knock onset. Moreover, turbulence-induced dispersion
534 promoted reaction rate increase of the unburnt mixture in this region, making it also the highest probability
535 knock location. An overall fraction of 66% of knocking cycles is calculated, which is in close agreement
536 with the experimental 63%.

537 The use of a PDF-based model allows to give a quantitative estimation of the knock probability events
538 associated with an average knock occurrence condition. The statistical model is based on transport equations
539 for the variance of physical conditions (enthalpy and mixture fraction) and tracks their variability in terms of
540 knock onset variance. The presented PDF-based knock model combines both the accuracy of a detailed
541 chemical mechanism used to calculate the autoignition delay times and the applicability of a RANS-based
542 model. The presented model aims at filling the existing gap between the scarcely representative average
543 knock prediction given by traditional RANS models and the cycle-resolved knock simulation possible with
544 CPU-intensive multi-cycle LES simulations. The combination of RANS models with variance transport
545 equations allows to quantify the probability of knocking events given by turbulence-originated fluctuation of
546 end-gas pockets, and it allows RANS simulations to be directly correlated with engine test-bench acquisition.

547

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618 Abbreviations

AI	Autoignition
aSOC	After Start of Combustion
aTDC	After Top Dead Centre
BDC	Bottom Dead Centre
bTDC	Before Top Dead Centre
CA	Crank Angle

CCV	Cycle-to-Cycle Variability
CDF	Cumulative Distribution Function
DI	Direct Injection
DKI	Dimensionless Knock Indicator
FSD	Flame Surface Density
GDI	Gasoline Direct Injection
IMPO	Integral Modulus of Pressure Oscillations
KLSA	Knock Limited Spark Advance
KO	Knock Onset
LES	Large-Eddy Simulation
MAPO	Maximum Amplitude of Pressure Oscillations
MFB	Mass Fraction Burnt
PDF	Probability Density Function
RANS	Reynolds-Averaged Navier- Stokes
RMS	Root Mean Square
SA	Spark Advance
SI	Spark Ignition
SOI	Start of Injection
TDC	Top Dead Centre
TRF	Toluene Reference Fuel