

Document downloaded from:

<http://hdl.handle.net/10251/142515>

This paper must be cited as:

López, JJ.; García-Oliver, JM.; García Martínez, A.; Villalta-Lara, D. (05-0). Development of a soot radiation model for diesel flames. *Applied Thermal Engineering*. 157:1-10.
<https://doi.org/10.1016/j.applthermaleng.2019.04.120>



The final publication is available at

<https://doi.org/10.1016/j.applthermaleng.2019.04.120>

Copyright Elsevier

Additional Information

1 **Development of a Soot Radiation Model for Diesel flames**

2 **Authors:**

3 J.J. López, J.M. García-Oliver, Antonio García, David Villalta

4 **Affiliation:**

5 CMT Motores Térmicos – Universitat Politècnica de València, Camino de Vera s/n,
6 46022, Valencia, Spain.

7 **Corresponding Author:**

8 Dr. Antonio García

9 CMT - Motores Térmicos /Universitat Politècnica de València

10 angarma8@mot.upv.es

11

12

13

14

15

16

17

18

19

20 **HIGHLIGHTS**

21 Radiation model is based on two sub-models: spray model and soot model.

22 The spray model estimates a penetration very similar to the experimental values.

23 Soot Yield concept combines the soot formation and oxidation processes.

24 Higher radiant fraction value is obtained when the oxygen molar fraction is reduced.

25 The radiant fraction shows values from 0.11% to 0.43% respect to the total fuel energy.

26 **KEYWORDS**

27 Radiation; soot; heat transfer; spectral intensity; soot radiation model

28 **ABSTRACT**

29 This paper describes a radiation model for diesel sprays that can predict the heat losses
30 based on spray characteristics to the spray plume due to radiation. The model is based on
31 three sub-models: spray model, soot model and radiation model. The spray model is a
32 one-dimensional model that simulates the axial and radial distribution of a fuel spray for
33 each instant. The soot model is a one-dimensional tool, which is based on formation and
34 oxidation processes calculating the axial and radial soot concentration profile for each
35 instant. The output results of the two sub-models are used as input information for the
36 radiation model, which obtains the radiation heat transfer values for a diesel flame. The
37 experimental measurements used to adjust the different constants and to validate the sub-
38 models were performed in a high-pressure high-temperature vessel using three different
39 optical techniques: Schlieren, to obtain spray penetration, Diffused Back-Illumination
40 technique (DBI) for the soot concentration and the 2-color method for calculating the soot
41 temperature and concentration. The radiant fraction shows values from 0.11% to 0.43%
42 with respect to the total energy of the fuel depending on the operating condition. Taking

43 into account the different assumptions taken for modeling the spray radiation, these
44 results are consistent with those obtained in the literature, in which the radiation was
45 characterized under similar conditions.

46 **1. INTRODUCTION**

47 Radiation heat transfer plays an important role in the heat transfer in direct-injection (DI)
48 diesel engines, being a significant component of the efficiency losses in modern designs.
49 Rough estimates of the heat transfer in the combustion chamber for the whole engine
50 cycle show that radiation varies from 0.5-1 % [1] up to 5-10 % [2] of the total fuel energy
51 depending on soot conditions (concentration and temperature). This value differs
52 significantly depending on the geometry of the combustion chamber, fuel used, operating
53 conditions, etc.

54 The main source of thermal radiation are soot particles, which emit radiation over the
55 entire wavelength spectrum. It is worthy to note that radiation is also emitted by CO₂ and
56 H₂O molecules but it is concentrate in a narrow spectral bands and its magnitude is
57 assumed to be much smaller than that of soot particles [3]. Soot formation is a complex
58 process comprising several physical and chemical phenomena, some of which occur
59 simultaneously, and depends largely on local conditions. Computational models typically
60 include processes such as precursor formation, particle inception, surface growth and
61 particle oxidation. These models have typically been developed for use with CFD diesel
62 engine models, but with a lower simulation cost. Regarding its use, soot emissions have
63 been analyzed in different studies: for varying the injection timing [4], different oxygen
64 concentrations in the intake air [5], adding post injection event [6] , etc. Deep knowledge
65 of the processes that include soot particles is important for two main reasons: on the one

66 hand, soot emissions are limited by strict pollutant regulations. On the other hand, soot
67 particles are mainly responsible for the total radiation heat transfer in diesel engines [7].
68 The main objective of this investigation is to develop a soot radiation model that it is able
69 to predict the radiation heat losses. This study is based on the distribution of soot inside
70 the flame, as well as understanding the processes that affect the radiation heat losses. For
71 that, three sub-models have been used: spray model, which includes all the fundamental
72 knowledge about combusting diesel sprays, a soot model, including both the formation
73 and oxidation processes, and a radiation model. The radiation model simulates the
74 temporal evolution of the spectral intensity, and consequently, the total soot radiation
75 losses from the simulated soot concentration results.

76 **2. EXPERIMENTAL DATABASE**

77 Throughout this study, experimental results previously published in [8] have been used
78 to calibrate the different constants for each model. Post-processing has been adapted to
79 compare with the simulated results in the different models. Next, the experimental facility
80 used for the experimental measurements and the test conditions are described.

81 **2.1. Experimental set-up: High pressure and high temperature vessel**

82 The high pressure and high temperature (HPHT) vessel is an experimental facility, that
83 allows to replicate engine like thermodynamic conditions to a diesel engine at the instant
84 of injection (Figure 1). The vessel is classified as a constant-pressure flow (CPF) facility
85 [9] as the conditions are reached by a continuous flow of high-pressure high temperature
86 gas through the vessel. The vessel is equipped with three large optical accesses (128 mm
87 in diameter) arranged in an orthogonal manner so that there is a full vision of the spray
88 plume. The mechanical limits of the vessel are 15 MPa of gas pressure and 1000 K of gas
89 temperature, and it is possible to obtain nearly quiescent and steady thermodynamic

90 conditions in the vessel. A common rail injection system allows changing the fuel
91 injection pressure and the duration of injection.



92

Figure 1. High pressure and high temperature vessel [9]

93

94 The pressurized gas is supplied to the vessel by two volumetric compressors working in
95 parallel, providing a continuous feed of 70 Nm³/h. The vessel can work in open or closed
96 loop to test spray evolution either in a standard air atmosphere or in gas mixtures with
97 different O₂ concentrations.

98 To heat the air, two electrical heaters of 15 kW each are placed upstream the vessel. A
99 secondary 2.5 kW heater is placed at the bottom of the chamber to help maintain the
100 temperature. Additionally, a 3 kW heating liner is placed in the periphery of the vessel to
101 minimize the heat losses from the ambient air.

102 **2.2. Previous experimental results**

103 The test matrix is conformed of six operating conditions from a previous study [8]. These
104 operating conditions are based on ECN-Spray A reference conditions, using n-dodecane
105 as fuel. The injection pressure was swept (500, 1000 and 1500 bar) as well as the O₂ molar
106 fraction (15 and 21%) keeping the density constant at 22.8 kg/m³ and the bulk gas
107 temperature at 900 K.

Temperature [K]	Density [kg/m ³]	Injection pressure [bar]	Molar fraction O ₂ [%]
900	22.8	500 / 1000 / 1500	15 / 21

Table 1. Operating conditions

108

109 A single-hole piezoelectric injector was used with a nominal diameter nozzle of 90 μm .

110 The energizing time (ET) of the injector was set at 2 ms for all conditions, which results

111 in a 3.5 ms hydraulic duration. Each measurement consisted on 10 repetitions in order to

112 reduce the experimental measurement uncertainties.

113 The operating conditions were measured by three different optical techniques:

114 • Schlieren optical technique [10]: a conventional Schlieren single-pass

115 arrangement was employed to detect the complete spray boundaries at high

116 temperature and high pressure conditions. Schlieren imaging technique enables to

117 detect gradients in the refractive index of a transparent medium. The technique

118 relies on the deviation of a light beam produced when light passes through non-

119 homogeneous fluids. For this study, this optical technique has been used to obtain

120 spray penetration.

121 • Diffused Back-Illumination technique (DBI) [11]: as an extinction-based

122 diagnostic, the soot volume fraction is related to the amount of light that has been

123 absorbed or scattered by the soot cloud. For this work, the temporal and spatial

124 soot concentration (KL) are obtained by DBI technique to compare with the

125 modelled soot concentration results.

126 • 2-color method (2C) [12]: it is an optical thermometry technique that makes use

127 of the presence of soot within a flame. It is particularly useful for diesel

128 combustion studies due to the fact that soot incandescence dominates the flame

129 radiation emission during most of the heat release period. In this sense, flame

130 images recorded by means of conventional visualization techniques in the visible

131 spectrum are basically soot radiation images. In this work, the 2-color method was
132 used to calculate the soot temperature and concentration.

133 **3. METHODOLOGY**

134 The structure of the complete radiation model is shown in Figure 2. Three sub-models,
135 which are directly connected to each other, compose the whole model. The spray model
136 (named DICOM) is a one-dimensional model that simulates the axial and radial
137 distribution of a fuel spray for each instant. This model needs input variables such as the
138 temporal evolution of the ambient pressure, ambient density, injection rate and the spray
139 angle that is necessary to calibrate with experimental data. For this, the experimental
140 results of spray penetration in both inert and reactive environment measured with the
141 Schlieren technique will be used to adjust the spray angle parameter (Section 4.3).

142 Once the spray model has been calibrated, these spray model results have been used as
143 input variables for the soot model and thus, axial and radial profiles of soot mass fraction
144 have been obtained for each instant. As in the spray model, in the soot model the optimal
145 values for two constants (K_{soot} and T_0) need to be adjusted from experimental results of
146 soot concentration (Section 5.2). These experimental results have been measured with the
147 Diffused Back-Illumination technique (DBI). In the next step, the temporal evolution of
148 the spectral intensity has been obtained from the simulated soot concentration results
149 together with the spatial temperature distribution calculated also in the spray model
150 (Section 6.3). Finally, the simulated spectral intensity is integrated for the whole
151 wavelengths spectrum and the radiation heat losses are obtained. As in two previous
152 models, the simulated radiation has been compared with experimental values from the 2-
153 Color method.

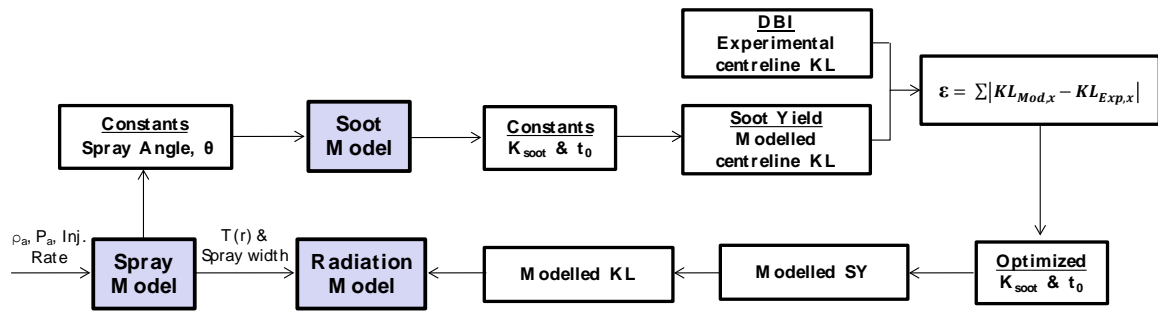


Figure 2. Overall model structure

4. SPRAY MODEL

Currently, there are several computational models capable of analyze and characterize the internal diesel spray structure in an injection/combustion process with temporal and spatial resolution. The set of computational tools ranges from complex models (known as 3D CFD) to more simplified models in which certain assumptions are made. In this work a one-dimensional model has been selected, which adapts perfectly to requirements of the analysis and has a short calculation time.

4.1. Spray model description

The spray model is a one-dimensional model capable of simulating the temporal and radial evolution of a fuel spray for inert (evaporative or non-evaporative) and reactive conditions, as well as for steady and transient conditions. This model has been developed by the CMT - Motores Térmicos group of the Universidad Politécnica de Valencia. This model is described in more detail in previous works [13][14].

The model approaches the analysis of a fuel spray injected through a single hole inside a closed volume, where the process of air/fuel mixing and the combustion processes are reproduced. The spray evolution is considered free of any spatial restriction and the closed volume is considered wide enough so that the air conditions remain constant.

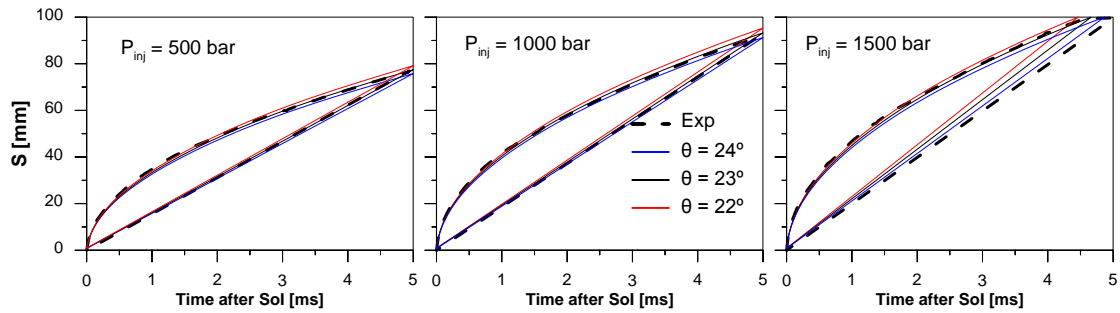
173 The model requires certain experimental data such as the temporal evolution of the
174 ambient pressure, the ambient density and the injection rate, injector properties (orifice
175 number, diameter, spray angle) and fuel. As output values, the model generates
176 comprehensive results, which describe the air/fuel mixture process with axial and
177 temporal resolution. These results are used as input values in the soot and radiation
178 models.

179 **4.2. Spray model calibration under inert conditions. Spray Angle**

180 As mentioned in section 3, the only unknown input of the model is the spray angle;
181 therefore, it needs to be determined by adjusting the results of the modelled vapor
182 penetration to the experimental Spray-A results, defined in table 1.

183 To validate the model and to determine the adequate spray angle for a given set of
184 conditions, a series of calculations were made at small angle increments (1°); then, the
185 deviation from the experimental curves was determined, and based on that, the value for
186 the angle was chosen. Figure 3 shows the experimental vapor penetration for the Spray-
187 A standard conditions and the curves for three different spray angles as predicted by the
188 model. It can be seen that a wider angle (24°) tends to under-predict the penetration, while
189 a narrower angle (22°) may seem more appropriate at the beginning of the spray, but at
190 the end, it overestimates the penetration values with respect to the experimental case. In
191 this case, the best match between experimental and simulation data was achieved at spray
192 angle of 23° .

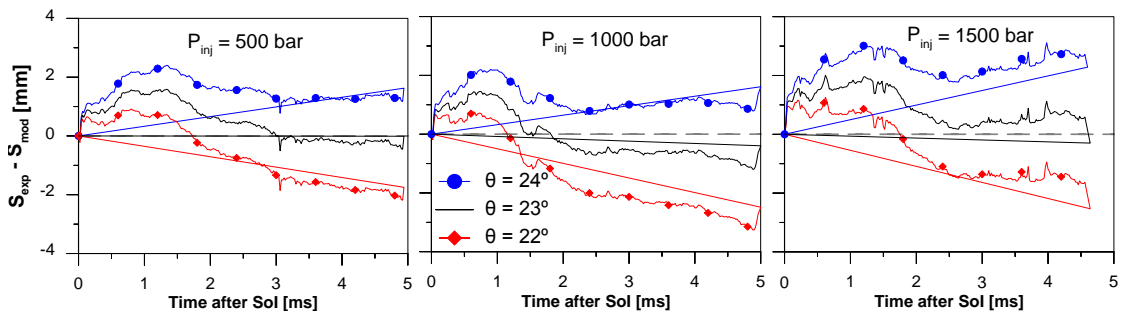
193



194

195 *Figure 3. Experimental and modelled vapor penetration for the three spray angles and different injection*
 196 *pressures tested under inert conditions*

197 Figure 4 shows the temporal evolution of the difference (in absolute values) between the
 198 experimental and modelled vapor penetration for the three spray angles tested and for the
 199 three different injection pressures. In addition, it has been found in the literature [15][16]
 200 that the spray angle depends mainly on ambient density and the injection pressure. In this
 201 investigation only the injection pressure has been varied. Although there are differences
 202 depending on the injection pressure, they are small to choose a different spray angle
 203 depending on the injection pressure. Therefore, the angle selected was 23° since it
 204 presented a good balance between the near and far regions of the spray from the nozzle.



205

206 *Figure 4. Difference between experimental and modelled vapor penetration for the three spray angles*
 207 *and different injection pressures tested under reactive conditions*

208

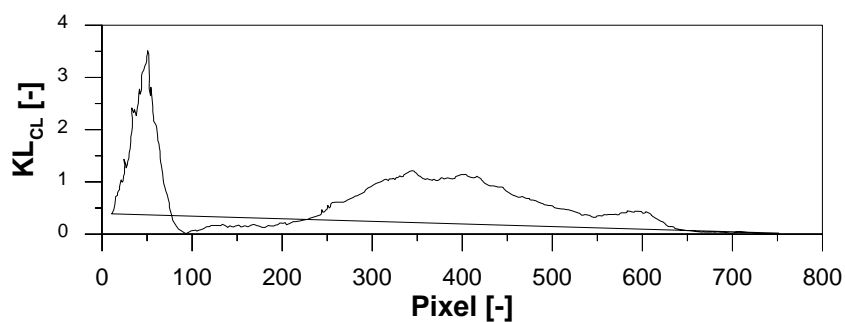
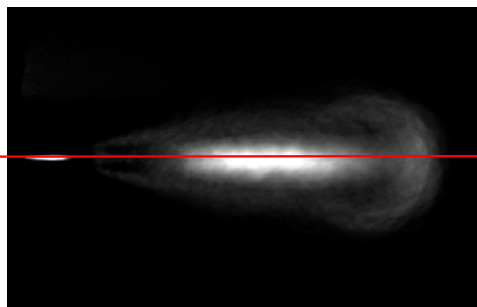
209 **4.3. Spray model validation under reacting conditions**

210 To determine the most suitable angle for the operating conditions measured, the model
 211 has calculated the vapor penetration under reactive conditions with the selected angle in

212 inert conditions (23°). The results obtained have been compared with the experimental
213 values for determining the most adequate spray angle.

214 Prior to the comparison, it is necessary to describe the methodology used to obtain the
215 experimental spray penetration from the images. The technique used to obtain spray
216 penetration was Diffused Back-Illumination technique (DBI). Each image corresponds to
217 a spatial distribution of the DBI signal (KL) every $100 \mu\text{s}$. The DBI signal distribution is
218 shown at the top image of Figure 5. To acquire the spray penetration, the DBI signal
219 values along the central axis have been plotted (bottom image of Figure 5), taking as
220 center line, an imaginary axis that comes from the center of the nozzle. For each image,
221 the furthest location on the axis where the DBI signal exceeds a threshold is defined as
222 the flame penetration. In this way, a temporal evolution of the flame penetration is
223 represented from the experimental images.

224

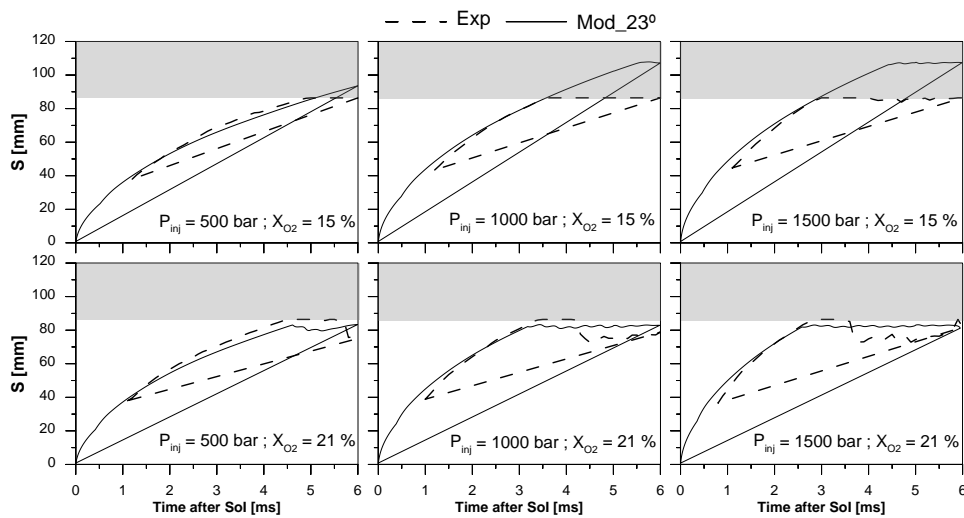


225

226 *Figure 5. Top) Spray image obtained from the Diffused Back-Illumination technique and bottom) the soot*
227 *concentration profile in the centerline.*

228 Figure 6 shows the temporal evolution of the experimental spray penetration (solid line)
229 and modelled (dashed line) for the six operating conditions analyzed. It should be noted

230 that there is a field of view limitation caused by the optical access of the vessel. Therefore,
 231 the maximum penetration able to be captured in the experimental measurements was 86
 232 mm. As shown in Figure 6, the temporal evolution of the flame penetration is split in two
 233 stages. First, one is the transient stage, in which the flame penetration increases
 234 progressively, where the modelled and experimental results show small differences (at
 235 least until the distance of 86 mm). The second is the steady stage where the flame
 236 penetration maintains a quasi-constant value (the flame front is stabilized). This phase
 237 can only be observed in 21% oxygen results due to the above-mentioned limitation in
 238 optical access. For lower oxygen concentration, stabilized flame penetration extends to
 239 approximately 110 mm [17]. The flame penetration in the steady zone presents slight
 240 differences (around 5 mm), which is due to a deviation from the acceptable experimental
 241 values. Thus it is possible to conclude that, at least for the whole conditions used in this
 242 study, the most suitable spray angle is 23°.



243

244 *Figure 6. Experimental and modelled spray penetration under reactive conditions for the six conditions*
 245 *tested.*

246 5. SOOT MODEL

247 In this section a one-dimensional soot model is presented. This model considers both soot
248 formation and oxidation processes. The model uses the calculated results in the one-
249 dimensional spray model as input variables, thus obtaining axial and radial soot
250 concentration profiles for each instant in a diesel flame. In a first section, the model will
251 be described along with the equations. Then, the necessary constants will be adjusted
252 from the experimental results. Finally, the model will be validated with experimental data.

253 5.1.Soot model description

254 The soot model is based on Monin's study [19]. In this work, a parameter was proposed
255 to model the soot formation process easily. The parameter was referred to as “soot yield”
256 (SY) and is defined as the ratio between the mass fraction of fuel transformed into soot
257 (Y_{soot}) and the mass fraction of unburned available fuel at that location (Y_{f_nb}):

$$258 \quad (1) \quad SY = \frac{Y_{soot}}{Y_{f_nb}}$$

259 It is important to define non-burned fuel mass fraction parameter for each instant and
260 flame location. This mass includes all the mass coming from the unburned fuel that is
261 available in that location with no distinction of its state (original fuel, cracked fuel, partly
262 oxidized fuel or soot). This parameter is an input value to the soot model from the spray
263 model (mixing/combustion).

264 Later, López et al. [20] proposed a correlation for the SY:

$$265 \quad (2) \quad SY = K_{soot} \cdot \max\left(0.5 - \frac{1}{Fr_{LOL}}, 0\right) \cdot t_r \cdot \exp\left(\frac{T_0}{T_{Flame}}\right) \cdot \rho^{2.2}$$

266 where Fr_{LOL} is the fuel-air equivalence ratio at the lift-off length, t_r is the residence time
267 inside the flame, T_{Flame} is the flame temperature, ρ is the ambient density and K_{soot} and T_0
268 are constant and their values have been fitting from experimental values (section 5.2).

269 • As many other researchers have observed [5][21] the soot formation process is
270 mainly controlled by the fuel-air equivalence ratio at the lift-off length. Usually,
271 a fuel-air equivalence ratio (Fr_{LOL}) of 2 is the limit to define whether soot is
272 produced (Fr_{LOL} higher than 2) or not (Fr_{LOL} lower than 2) in a combusting diesel
273 spray. For this reason, the soot yield is assumed to be different from this value.
274 Finally, the Fr_{LOL} is an input variable to the soot model calculated by the spray
275 model (mixing/combustion).

276 • The soot formation also depends on the residence time of the fuel inside the fuel-
277 rich region of the reacting spray. The residence time parameter is defined as
278 $t - t_{LOL}$, where t is the instant under study and t_{LOL} stands for the time at which the
279 considered fuel reaches the lift-off length. The SY is proportional to t_r . As it is
280 well known, an increase in temperature at the lift-off length implies an
281 improvement in soot formation. Monin [19] assumed that this parameter affects
282 exponentially the rate of soot formation process: $\exp(T_0/T_{Flame})$, where T_0 is a
283 constant obtained from comparison with experimental results.

284 • Finally, Pickett found that the soot formation process is also affected by the
285 ambient pressure (or, for a given temperature, by density) [21]. Based on the data
286 published in his work, the corresponding function is the following: $\rho^{2.2}$, which also
287 should affect the soot yield.

288 Once the factors, the SY parameter depends on, are defined from the product of equations
289 (1) and (2) the mass fraction of soot, Y_{soot} , can be obtained. Nevertheless, both two and
290 both most common soot measuring techniques (DBI and two-color method) provide a

291 value for X_{soot} (volume fraction). Consequently, the conversion from one magnitude to
292 the other is required. This conversion can be done as follows:

$$293 \quad (3) \quad X_{soot} = Y_{soot} \cdot \frac{\rho_a}{\rho_{soot}}$$

294 where ρ_{soot} is the density of the soot particles and ρ_a is the density at the point under
295 consideration (local density). The soot particle density does not have a universal value.
296 However, some authors take a value of approximately 1800 kg/m^3 as a representative
297 value [22]. For the local density estimation, the local temperature and the mean pressure
298 are considered, assuming standard air for the constant in the equation of state.

299 Up to now, the soot model is able to predict the evolution of X_{soot} at the spray centerline.
300 As soot radiation takes place at any region where temperature is sufficiently high, the
301 value of the soot volume fraction at any other point of the spray section is needed. There
302 is not much information available in the literature about the shape of the X_{soot} radial
303 profile. For this model, a Gaussian profile has been chosen to simulate the flame section,
304 similar to mixture fraction profiles as in [24], which follows the following equation:

$$305 \quad (4) \quad \frac{X_{soot}}{X_{soot,CL}} = \exp \left[-4.6 \cdot \left(\frac{r}{R_{Flame}} \right)^2 \right]$$

306 where r is the radial coordinate and R_{Flame} the flame radius at the section under
307 consideration.

308 **5.2. Adjustment methodology. Soot model validation**

309 This section describes the calibration of the model constants, K_{soot} and T_0 , and the soot
310 model validation. For both objectives, experimental results of the soot concentration from
311 the Diffused Back-Illumination technique (DBI) were used.

312 The flow chart in Figure 7 describes the methodology used to calibrate the constants K_{soot}
 313 and T_0 is shown. These two parameters have been found by searching the lowest error
 314 when comparing the experimental and the modelled soot concentration at each axial and
 315 radial position. This procedure was divided into several steps:

- 316 • First, an initial value is assigned to each constant. With them, the parameter SY is
 317 calculated. As described in section 5.1, a soot molar fraction value (X_{soot}) is
 318 obtained for each flame axial and radial position. Next, the soot concentration
 319 values (KL) is calculated from the information of the soot model and compared
 320 with the experimental values provided by the DBI method. The conversion of X_{soot}
 321 to KL is based on the Beer-Lambert equation, which evaluates the light
 322 attenuation [18]:

$$323 \quad (5) \quad \frac{I}{I_0} = \exp(-KL) = \tau$$

324 where I_0 is the incident light intensity, I is the attenuated light intensity and τ , the
 325 transmissivity. If it is considered that the flame is divided radially into n elements
 326 with the same thickness, the equation (5) can be rewritten as follows:

$$327 \quad (6) \quad \frac{I}{I_0} = \exp(-KL) = \tau = \sum_{i=1}^n \tau_i$$

328 where τ_i represents the transmissivity of each portion of the spray. According to
 329 Musculus [18], the transmissivity is related to the soot volume fraction in the
 330 following way:

$$331 \quad (7) \quad \tau_i = \exp\left(\frac{-g \cdot X_{\text{soot}}(r) \cdot dr}{\lambda^\alpha}\right)$$

332 where g is a constant equal to $6.3 \mu\text{m}^{-1}$, λ is the wavelength in μm and $\alpha = 1.22$ -
 333 $0.245 \cdot \ln(\lambda)$, with λ in μm and dr is the thickness for each element. If equations

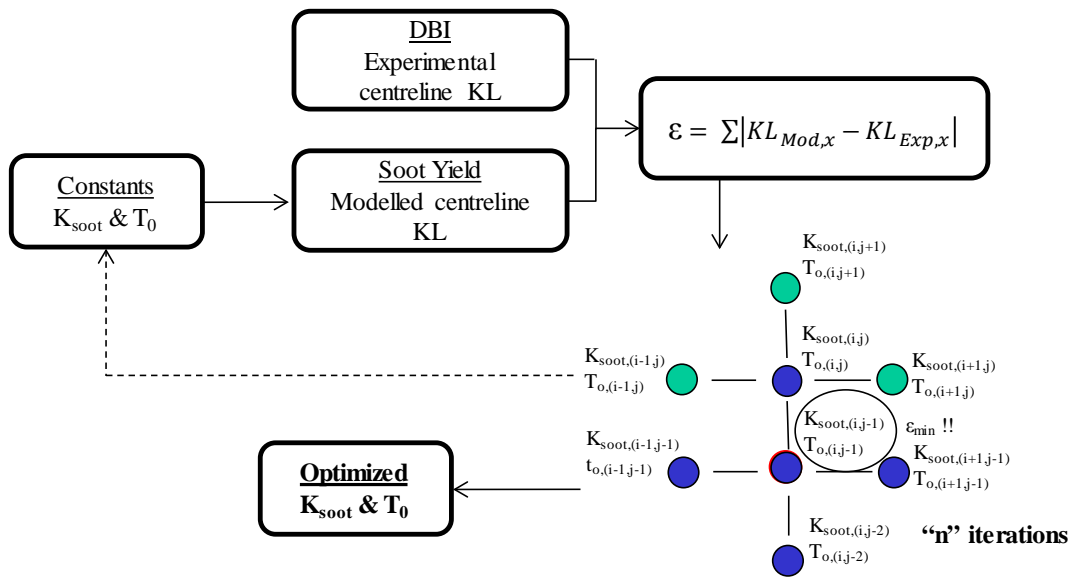
334 (6) and (7) are considered together, and it is taken into account that the product of
335 an exponential is the exponential of an addition, it can be seen that KL can be
336 related to the local conditions in the following way:

337 (8)
$$KL = \frac{g}{\lambda^\alpha} \cdot \int_{-L/2}^{+L/2} X_{soot}(r) \cdot dr$$

338 To finish this first step, the difference (ε) of the modelled and experimental soot
339 concentrations for each axial and radial position is calculated.

340 • The second stage consists of performing the same previous procedure until
341 reaching the sum of the differences, but in this case varying the values of both
342 constants. In particular, both constants were varied $\pm 20\%$ of their initial value.
343 This indicates that the first step is repeated with all possible combinations of the
344 constants, that is, four times.

345 • Finally, the constant combination with lower value is chosen from the five error
346 results (initial + 4 combinations). This pair of constants are considered as initial
347 values and the whole procedure is repeated, so that finally a matrix with five
348 accumulated errors corresponding to five constant pairs is obtained again. This
349 step is repeated until the minimum error is achieved twice times consecutively by
350 the same constants K_{soot} and T_0 .



351

352

Figure 7. Experimental methodology used to fit/adjust the soot model constants (K_{soot} and T_0).

353

Considering the six operating conditions described in the test plan section, the values

354

obtained for the constants K_{soot} and T_0 are $11.25 \cdot 10^{-4}$ and 4687.5 K, respectively. Figure

355

8 shows the axial evolution of the experimental and modelled soot concentration along

356

the flame centerline at a given instant. The model adjusts the start and end of the flame

357

precisely. Qualitatively, the modelled results show good agreement with experimental

358

data (KL decreases when the injection pressure increases and/or the oxygen concentration

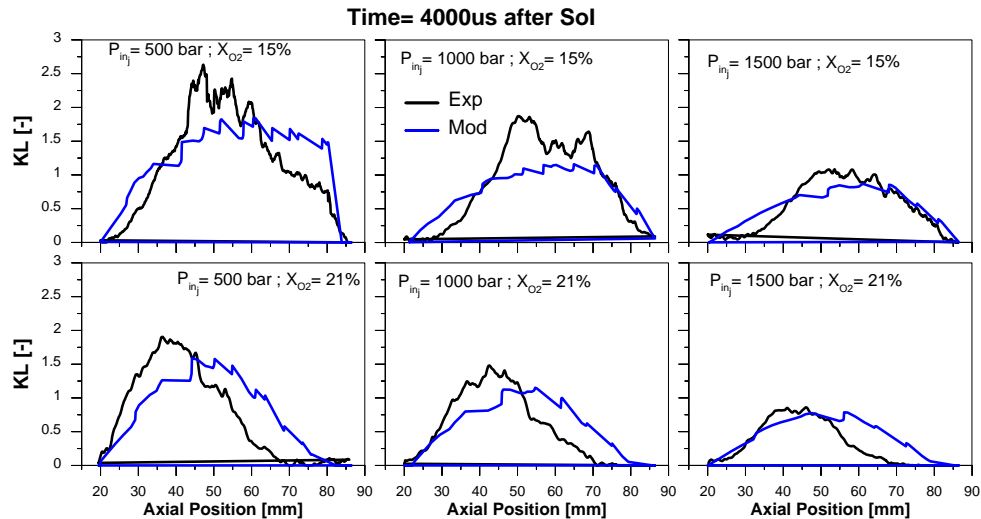
359

increases). Therefore, it is concluded that the soot model is correctly calibrated respect to

360

the experimental data.

361



362

363

Figure 8. Experimental and modelled soot concentration for six operating conditions.

364

6. RADIATION MODEL

365

This section presents the radiation model and the methodology to validate the model. For

366

that, the spectral intensity of the radiation (I_{soot}) has been calculated and compared to the

367

experimental values measured by the 2-color method. Then, the total radiation emitted by

368

the soot is calculated.

369

To begin with, these are the different assumptions taken for modeling the spray radiation:

370

- The spray/wall interaction will not be considered. Consequently, a free spray is considered.

371

372

- The swirl existing in the combustion chamber does not modify the spray geometry, which remains axisymmetric.

373

374

- The radiation is diffuse and it radiates in the same way in all directions.

375

6.1. Model description

376

The radiation intensity is the main output variable of the radiation model (as shown in

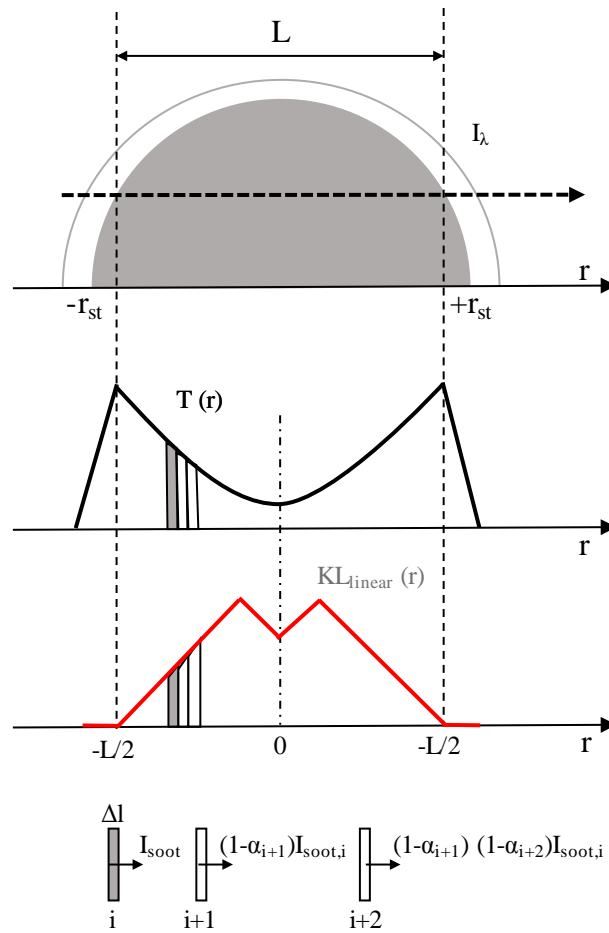
377

Figure 2) and this has been used as a basis to validate the present radiation model. The

378 radiation intensity in the radial direction has been calculated as explained by Payri *et*
379 *al.*[25].

380 Figure 9 presents the modelled combustion temperature and soot distribution for a
381 particular axial position. The temperature distribution has been obtained from the spray
382 model, as a function of the equivalence ratio distribution at each radial and axial position.
383 Three different zones can be observed in the temperature distribution: 1) the flame limits
384 are the stoichiometric surface, where the maximum temperatures are reached; in this
385 location the fuel diffused from the inner part of the flame reacts with oxygen from the
386 outer part. 2) the inner zone, which corresponds to the rich side of the flame; this region
387 consists of partially oxidized fuel, combustion products and soot. 3) the outer part, which
388 is the lean side of the flame; in this region fresh air and combustion products are present.
389 In terms of soot concentration, a linear distribution has been considered in which it is
390 assumed that the soot particles are only present in the inner part of the flame, as they are
391 totally oxidized by the OH present on the reaction zone [26].

392 The flame is divided radially into discrete flame elements with their corresponding values
393 of temperature and soot concentration. To analyze the radiation propagation inside the
394 flame, both emission and absorption processes have been considered.



395

396

Figure 9. Scheme radiation propagation through of the diesel spray [25]

397 Considering the temperature and soot distributions, the radiation propagation process
 398 inside the flame is based on the following:

- 399
- Radiation is propagated along lines parallel to the flame main symmetry plane.
 - 400 • The spatial distribution of the local gas temperature is assumed to be equal to the
 401 soot temperature. In this case, the spray model calculates the flame temperature.
 - 402 • Soot is assumed to be completely oxidized at the flame stoichiometric surface.

403 The radiation path is divided into n elements with the same thickness. Each element i has
 404 its temperature T_i and optical thickness KL_i . So, considering the proposed soot
 405 distributions it can be stated that:

406 (9) $KL = \sum_{i=1}^n (KL)_i$

407 As indicated in the description of the 2-color method [12], the radiation emitted by each
 408 element can be calculated as:

409 (10) $I_{soot,i}(\lambda, T_i, KL_i) = \varepsilon_{\lambda,i} I_b(\lambda, T_i)$

410 where ε indicates soot spectral emissivity and I_b corresponds to a blackbody spectral
 411 intensity. The radiation received by the sensor (which is located on either flame limits) at
 412 each wavelength is the addition of the $I_{soot,i}$ of each flame element. Considering the
 413 attenuation factor between elements, the total soot radiation intensity for each wavelength
 414 can be calculated as:

415 (11) $I_{soot,i}(\lambda, T_i, KL_i) = \sum_{i=1}^n [\varepsilon_{\lambda,i} I_b(\lambda, T_i) \cdot \prod_{j=i+1}^n (1 - \alpha_{\lambda,j})]$

416 where for an element j the absorption ($\alpha_{\lambda,j}$) is defined by the spectral absorptivity ($\varepsilon_{\lambda,j}$)
 417 as stated by Kirchhoff's law:

418 (12) $\alpha_{\lambda,j} = \varepsilon_{\lambda,j}$

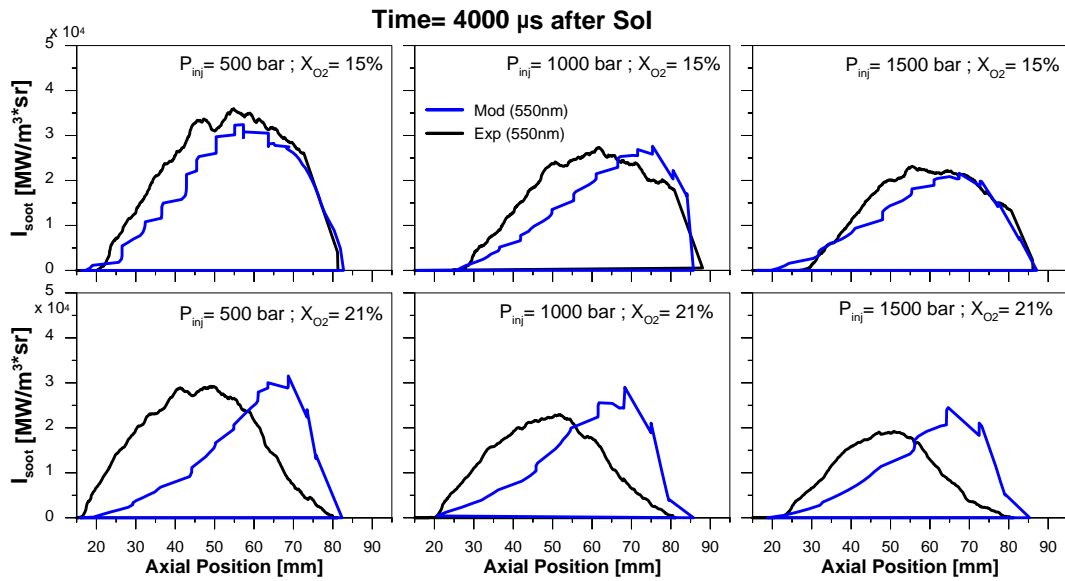
419

420 6.2. Spectral intensity

421 The purpose of this section is to evaluate the soot spectral intensity (as an output
 422 parameter of the radiation model) versus the experimental results from the 2-color
 423 method.

424 Figure 10 shows the axial evolution of the experimental and modelled soot spectral
 425 intensity along the centerline for the six operating conditions. The soot spectral intensity
 426 has been calculated for two wavelengths, $\lambda = 550$ and 650 nm. For simplicity, only the
 427 results for $\lambda = 550$ nm are shown. In general, both modelled and experimental soot
 428 spectral intensity values decrease when the injection pressure increases and/or the oxygen

429 mass fraction increases. By comparing each graph individually, it can be established that
 430 the model provides a good accuracy during the onset of the flame. If the flame length is
 431 divided into two parts, in the first one, the model sub-predicts the soot spectral intensity
 432 values. This phase is estimated up to 60-70 mm from the injector. From this, the trend
 433 changes and the model over-predicts the results respect to the experimental results.



434

435 *Figure 10. Experimental and modelled soot spectral intensity along the spray centerline for the six*
 436 *operating conditions.*

437 **6.3. Total radiation**

438 The next step in the validation of the radiation model is the calculation of the total
 439 radiation emitted by soot particles. Based on the soot spectral intensity, the total radiation
 440 was obtained from the integration of the spectral intensity for a particular range of
 441 wavelengths using equation (13):

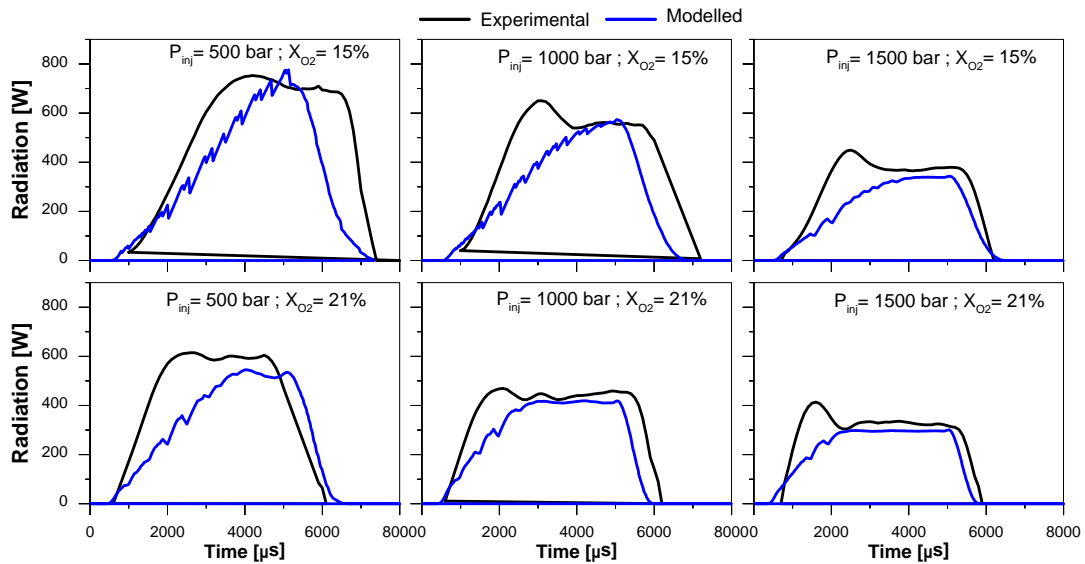
$$442 \quad (13) \quad Q_{rad} = \pi \int_t \int_A \int_\lambda \varepsilon_\lambda I_{b,\lambda} d\lambda dA dt$$

443 where t represents the exposure time in which the optical system is registering flame
 444 luminosity, and A is the flame area obtained by equation (14):

445 (14)
$$A_t = 2\pi r \int_x dx$$

446 where r is the flame radius, which is determined from a temporal image of the flame, and
 447 dx is the axial width.

448 Figure 11 represents the temporal evolution of the experimental and modelled total
 449 radiation for the six operating conditions studied. For the six cases analyzed, the model
 450 predicts total radiation values similar to the experimental. Considering the simplifications
 451 and assumptions of each model, the results shown in Figure 11 can be considered as
 452 acceptable results.



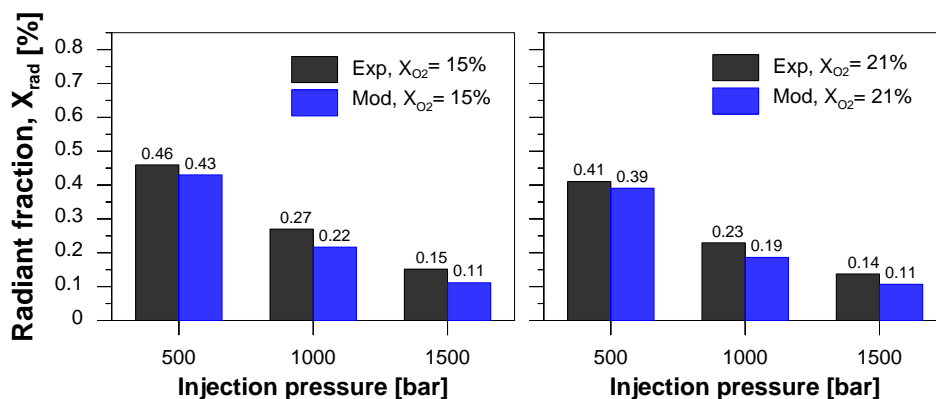
453
 454 *Figure 11. The temporal evolution of the experimental and modelled total radiation for the six operating*
 455 *conditions studied.*

456 Finally, to better quantify the total radiation, the radiant fraction has been calculated. The
 457 radiant fraction (X_{rad}) emitted by soot is defined as the fraction of the total chemical
 458 energy released during injection that is lost due to radiation heat transfer. This term is
 459 expressed by equation (15):

460 (15)
$$X_{rad} = Q_{rad} / m_f Q_{LHV}$$

461 where m_f represents the mass of fuel injected and Q_{LHV} is the lower heating value of
462 dodecane (44.2 MJ/kg).

463 Figure 12 shows the results of the radiant fraction emitted by soot for the different
464 operating conditions analyzed. Particularly, the sub-figure on the left shows the values of
465 radiant fraction modifying the injection pressure at oxygen molar fraction of 15% and,
466 the figure on the right, at oxygen molar fraction of 21%. Considering the results obtained
467 from soot concentration and spectral intensity in previous figures, the trends of radiant
468 fraction are expected. Thus, a reduction of injection pressure and/or oxygen molar
469 fraction implies a higher radiant fraction value. In addition, as in the previous graph of
470 the total radiation, the modelled radiant fraction values are slightly lower than the
471 experimental ones. Finally, the modelled radiant fraction values are between 0.11 and
472 0.43% respect to the total fuel energy. Comparing them with the results obtained from the
473 radiant fraction in [5], the modelled values are in the same order of magnitude.
474 Considering that the operating conditions are similar, the modelled results are coherent
475 with those obtained in [5]. This makes the radiation model a completely suitable tool to
476 predict and study the radiation heat transfer.



477

478 *Figure 12. Experimental and modelled radiant fraction modifying injection pressure and oxygen molar*
479 *fraction.*

480

7. CONCLUSION

481

In this study, a radiation model for diesel spray has been developed. This model is able

482

to predict the radiation from spray plume. The model is based on three sub-models: a

483

spray model, which analyzes and characterizes the internal spray structure in terms of

484

mixing and combustion process with temporal and spatial resolution. A soot model, based

485

on soot formation and oxidation processes. The cohesion of these two sub-models is used

486

to obtain the input values to the third model, the radiation model from which the radiation

487

heat transfer values for a diesel flame are obtained. The main contributions of this paper

488

are:

489

- The one-dimensional spray model has been adjusted for the only unknown

490

variable: the spray angle. For the cases analyzed here, the most suitable spray

491

angle has been found to be 23° comparing the penetration results in inert

492

conditions. Regarding the validation of the model, penetration values have been

493

used in reactive conditions. The model estimates a penetration very similar to the

494

experimental values, both in the transient and quasi-steady phases.

495

- The soot model is based mainly on the “soot yield” concept, which combines the

496

soot formation and oxidation processes depending on the time and location. This

497

model has been calibrated by means of two unknown constants: K_{soot} and T_0 . The

498

values of the constants are $11.25 \cdot 10^{-4}$ and 4687.5 K, respectively. These constants

499

have been obtained from an experimental methodology, where the soot

500

concentrations are compared with the experimental values measured by Diffused

501

Back-Illumination technique (DBI). The model predicts accurately the start and

502

end of the flame. Although in qualitative terms, the model accurately predicts the

503

experimental values. Depending on the axial position, the model sub-predicts or

504 over-predicts the experimental values. In general terms, the soot model matches
505 correctly with the experimental values.

506 • Finally, a methodology developed by Payri was used for the radiation model [25].
507 The methodology has considered both emission and absorption processes for
508 analyzing the radiation heat transfer inside the flame. From the soot concentration
509 estimated with the soot model and the soot temperature calculated from the spray
510 model, the modelled spectral intensity has been calculated. For the operating
511 conditions used in this study, the radiation model calculates radiant spectral
512 intensity values very similar to the experimental ones. Considering the
513 simplifications and assumptions of each model, it can be accepted as acceptable
514 results. The fraction of radiation shows values from 0.11% to 0.43% respect to the
515 total fuel energy depending on the operating condition. Considering the
516 differences in the operating conditions, these results are consistent with those
517 obtained in [5], in which the radiation was characterized under simplified
518 conditions. It is interesting to note that to determine the fraction of radiation, it is
519 only necessary to have the temporal evolution of the ambient pressure, the
520 ambient density and the injection rate, injector properties (orifice number,
521 diameter, spray angle) and properties of the fuel in addition to the boundary
522 conditions in which the operating conditions are tested. These experimental data
523 can be obtained quite easily.

524 **ACKNOWLEDGMENTS**

525 The authors acknowledge FEDER and Spanish Ministerio de Economía y Competitividad
526 for partially supporting this research through TRANCO project (TRA2017-87694-R).

REFERENCES

- 528 [1] P. Vogelín, Experimental investigation of multi-in-cylinder pyrometer
529 measurements and exhaust soot emissions under steady and transient operation of
530 a heavy-duty diesel engine, SAE technical paper 131ICE-0145; 2013.
- 531 [2] FJ. Struwe, In-cylinder measurement of particulate radiant heat transfer in a direct
532 injection diesel engine, SAE technical paper 2003-01-0072; 2003.
- 533 [3] P. Furmanski, J. Banaszek, T. S. Wisniewski, Radiation Heat Transfer In a
534 Combustion Chamber of Diesel Engine with Partially Transparent Burnt Gas Zone.
535 SAE Technical Paper 980504, 1988.
- 536 [4] D. Jung, D. Assanis, Multi-zone DI diesel spray combustion model for cycle
537 simulation studies of engine performance and emissions, SAE paper 2001-01-1246;
538 2001.
- 539 [5] X. Bi, H. Liu, M. Huo, C. Shen, X. Qiao, C. F.Lee, Experimental and numerical
540 study on soot formation and oxidation by using diesel fuel in constant volume
541 chamber with various ambient oxygen concentrations, Energy Conversion and
542 Management, Vol. 84, pp. 152-163, 2014.
- 543 [6] J. Benajes, J. Martín, A. García, D. Villalta, A.Warey, Swirl ratio and post injection
544 strategies to improve late cycle diffusion combustion in a light-duty diesel engine,
545 Applied Thermal Engineering, Vol. 123, pp. 365-376, 2017.
- 546 [7] J. Benajes, J. Martín, A. García, D. Villalta, A.Warey, In-cylinder soot radiation
547 heat transfer in direct-injection diesel engines, Energy Conversion and
548 Management 106, 414–427, 2015.

- 549 [8] S. Skeen, J. Manin, L. Pickett, E. Cenker et al., A Progress Review on Soot
550 Experiments and Modeling in the Engine Combustion Network (ECN), SAE Int. J.
551 Engines 9 (2), 2016.
- 552 [9] R. Payri, F.J. Salvador, P. Martí-Aldaraví, D. Vaquerizo, ECN Spray G external
553 spray visualization and spray collapse description through penetration and
554 morphology analysis, Applied Thermal Engineering, Vol. 112, pp. 304-316, 2017.
- 555 [10] R. Payri, J.M. Garcia-Oliver, T. Xuan, M. Bardi, A study on diesel spray tip
556 penetration and radial expansion under reacting conditions, Applied Thermal
557 Engineering, Vol. 90, pp. 691-629, 2015.
- 558 [11] J.V. Pastor, J.M. Garcia-Oliver, R. Novella, T. Xuan, Soot Quantification of Single-
559 Hole Diesel Sprays by Means of Extinction Imaging, SAE Int. J. Engines 8 (5),
560 2015.
- 561 [12] J. J. López, J. Martin, A. Garcia, D.Villalta, A. Warey, Implementation of two color
562 method to investigate late cycle soot oxidation process in a CI engine under low
563 load conditions, Applied Thermal Engineering, Vol. 113, pp. 878-890, 2017.
- 564 [13] J. V. Pastor, J. J. Lopez, J. M Garcia-Oliver, J. M. Pastor, A 1D model for the
565 description of mixing-controlled inert diesel sprays, Fuel, Vol. 87 no 13-14, pp.
566 2871-2885, 2008.
- 567 [14] J.M. Desantes, J.V. Pastor, J.M. García-Oliver, J.M. Pastor, A 1D model for the
568 description of mixing-controlled reacting diesel sprays, Combustion and Flame,
569 Vol. 156, pp. 234-249, 2009.
- 570 [15] J.V. Pastor, J.M. Garcia-Oliver, J.M. Pastor, W. Vera-Tudela, One-dimensional
571 diesel spray modeling of multicomponent fuels, Atomization and Sprays, Vol
572 25(2), pp. 485-517, 2015.

- 573 [16] E. Mancaruso, L. Sequino, B. Vaglieco, Analysis of spray injection in a light duty
574 CR diesel engine supported by non-conventioanl measurements, Fuel Vol. 158, pp.
575 512-522, 2015.
- 576 [17] D. Siebers, B. Higgins, L. Pickett, Flame Lift-off on direct-injection diesel fuel jets:
577 Oxygen concentration effects, SAE Technical Paper, n° 2002-01-0890, 2002.
- 578 [18] M. Musculus, Measurements of the Influence of Soot Radiation on In-Cylinder
579 Temperatures and Exhaust NOx in a Heavy-Duty DI Diesel Engine, SAE Technical
580 Paper, n° 2005-01-0925, 2005.
- 581 [19] C. Monin, Caracterización del Proceso de Formación de Hollín en una Llama de
582 Difusión Diésel de Baja Temperatura, Doctoral Thesis, 2009.
- 583 [20] J. López, J.M. Garcia-Oliver, J. Martin, J.P. Chemisky, A. Bouet, A Soot Radiation
584 Model for Diesel Sprays, SAE Technical Paper, n° 2012-01-1069, 2012.
- 585 [21] L.M. Pickett, D.L. Siebers, Soot in diesel fuel jets: effects of ambient temperature,
586 ambient density, and injection pressure, Combustion and Flame, vol. 138, pp. 114-
587 135, 2004.
- 588 [22] E. Mancaruso, S.S. Merola, B.M. Vaglieco, Study of the multi-injection
589 combustion process in a transparent direct injection common rail diesel engine by
590 means of optical techniques, Int. J. Engine Res. Vol 9, issue 6, pp. 483-498, 2008.
- 591 [23] D.F. Kronholm, J.B. Howard, Analysis of soot surface growth pathways using
592 published plug-flow reactor data with new particle size distribution measurements
593 and published premixed flame data, Proceedings of the Combustion Institute, vol.
594 28, pp. 2555-2561, 2000.
- 595 [24] J.M. Desantes, J. Arrègle, J.J. López, A. Cronhjort, Scaling laws for free turbulent
596 gas jets and diesel-like sprays, Atomization and Sprays, vol. 16, pp. 443-473, 2006.

- 597 [25] F. Payri, J.V. Pastor, J.M. García, J.M. Pastor, Contribution to the application of
598 two-colour imaging to diesel combustion, *Measurement Science and Technology*,
599 vol. 18, pp. 2579-2598, 2007.
- 600 [26] J. Dec, A Conceptual Model of DI Diesel Combustion Based on Laser-Sheet
601 Imaging, SAE Technical Paper 970873, 1997.