

Spray and Soot Formation Analysis by Means of a Quasi-Dimensional Multizone Model in a Single Cylinder Diesel Engine under Euro 4 Operating Conditions

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ABSTRACT

An investigation has been carried out on the spray penetration and soot formation processes in a research diesel engine by means of a quasi-dimensional multizone combustion model.

The model integrates a predictive non stationary 1D spray model developed by the Sandia National Laboratory, with a diagnostic multizone thermodynamic model, and is capable of predicting the spray formation, combustion and soot formation processes in the combustion chamber.

The multizone model was used to analyze three operating conditions, i.e., a zero load point (BMEP = 0 bar at 1000 rpm), a medium load point (BMEP = 5 bar at 2000 rpm) and a medium-high load point (BMEP = 10 bar at 2000 rpm). These conditions were experimentally tested in an optical single cylinder engine with the combustion system configuration of a 2.0L Euro4 GM diesel engine for passenger car applications.

The experimental spray tip penetration and spreading angle were evaluated on the basis of images acquired by means of a high-speed CCD camera, while the experimental trend of the in-cylinder soot concentration was derived by means of the two-color pyrometry method.

The acquired experimental data have allowed useful information to be obtained for the assessment of the multizone model. Well-defined trends between some of the model parameters and the engine operating conditions (namely, speed and load) have been found and preliminary correlations have been developed.

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INTRODUCTION

Zero-dimensional [1] and quasi-dimensional [2, 3, 4] multizone diagnostic combustion models for diesel engines have proved to be of fundamental importance in order to add useful information to the raw experimental results acquired at the test bench; these tools are capable of providing physical interpretations of the cause and effect relationships between the main engine calibration parameters and the combustion and pollutant formation processes.

They are in fact based on the discretization of the in-cylinder content into several zones, and they therefore allow an accurate prediction of the spray formation, temperature gradients and chemical composition of the different zones to be obtained, which in turn allows thermochemical and phenomenological submodels that evaluate the

formation of the main pollutant emissions to be implemented.

Single-zone diagnostic models [5] are in fact not capable of providing detailed information about in-cylinder thermodynamic processes, even though they are characterized by much faster computational times.

A quasi-dimensional multizone diagnostic combustion model has recently been developed by the authors for the analysis of the spray formation, combustion and emission formation processes in direct injection (DI) diesel engines [2, 3, 4]. The model is a refinement of a previous version that was presented in [1]. The main novelty consists of the integration of a predictive 1D spray model developed by the Sandia National Laboratory [6, 7], which is capable of evaluating the spray penetration and the average equivalence ratio of the spray as a function of the axial distance of the spray and of time. The latter quantity is fundamental for an accurate evaluation of the soot

formation process, which mainly depends on the local equivalence ratio dynamics during fuel/charge mixing and at the early stages of combustion [8].

The combustion process has been studied by means of a diagnostic approach, in which the heat release rate is derived from the measured in-cylinder pressure trace. The model is based on the splitting of the in-chamber content into several homogeneous zones, to which energy and mass conservation principles are applied. Several combustion conceptual schemes are adopted, starting from the Dec one [9], which has also been extended to highly premixed combustion cases [3]. Premixed and diffusive contributions to the heat release rate are taken into account. A post-combustion mixing and cooling submodel has been implemented in order to take into account the dilution of the burned gases produced from diffusive combustion. The latter has an important impact on the oxidation process of the in-cylinder pollutant emissions, and especially on soot. The main outcomes of the thermodynamic model are the temperature and mass evolutions of the different zones, along with their chemical composition. These quantities allow specific submodels to be implemented for the calculation of NO, CO, soot and THC [2].

The integration of a combustion diagnostic multizone approach with a non-stationary 1D spray model can be considered innovative compared to previous thermodynamic models [10, 11] that include a free, fully developed, quasi-steady fuel spray model [12]. The use of a non-stationary model to simulate the spray dynamics is of fundamental importance, because it allows the injection rate profile to be implemented directly as model input. It therefore allows the effects of the shape of the injection rate on the equivalence ratio distribution of the spray, as well as “entrainment wave” effects, such as those reported in [6], to be taken into account.

A preliminary assessment of the model was carried out in [4] on the basis of an experimental investigation which was conducted on an optical single-cylinder engine. In particular, the spray tip penetration and the in-cylinder soot concentration derived by means of the two-color pyrometry method were used for the calibration of the 1D spray model, of the soot formation model and of the burned gas dilution model. The analysis was carried out at low load (BMEP = 2 bar at 1500 rpm) and medium load (BMEP = 5 bar at 2000 rpm) operating conditions for an 8-hole solenoidal injector.

The same analysis has been carried out in this study for a zero load point (BMEP = 0 bar at 1000 rpm), a medium load point (BMEP = 5 bar at 2000 rpm) and a medium-high load point (BMEP = 10 bar at 2000 rpm), using a 7-hole solenoidal injector. This investigation has allowed the abovementioned models to be further refined, and preliminary trends between the model parameters and the engine operating conditions (namely, speed and load) to be identified.

MODEL DESCRIPTION

A detailed description of the multizone model is provided in [3], and as a result a detailed description of the methodology has not been given here for the sake of brevity. However, a summary of the method is reported in this section.

1D Spray Model

For a complete description of the 1D spray model, the reader should refer to [6, 7]. The model was developed in [6] for a non-vaporizing jet; however, it was shown in [7] that it is capable of correctly predicting the spray penetration and mixture fraction distribution also for vaporizing jets, under the assumption of mixing-limited vaporization.

The spray generated from each nozzle hole is considered as a conic-shaped region with a constant spreading angle θ . This region is discretized into several control volumes i , for which the transient transport equations for fuel mass m_f and axial momentum M are written:

$$\frac{\partial m_f}{\partial t} = \dot{m}_{f,in} - \dot{m}_{f,out} \quad (1)$$

$$\frac{\partial M}{\partial t} = \dot{M}_{in} - \dot{M}_{out} \quad (2)$$

It is assumed that the turbulent mean fuel volume fraction $\bar{X}_f$ and the turbulent mean velocity $\bar{u}$ vary along the radial coordinate of a generic cross section according to the following equations:

$$\frac{\bar{X}_f}{\bar{X}_{f,c}} = (1 - \xi^\alpha)^2 \quad (3)$$

$$\frac{\bar{X}_f}{\bar{X}_{f,c}} = (1 - \xi^\alpha)^2 \quad (4)$$

where $\xi = r/R$ is the ratio of the radial coordinate r to the maximum coordinate R , which is a function of the axial coordinate. c denotes the conditions on the jet centerline, and α is a parameter which accounts for the evolution from a top-hat shape at the nozzle exit ($\alpha = \infty$) to a fully developed shape ($\alpha = 1.5$).

It was shown in [6] that, when Eqs. (3), (4) are taken into account, it is possible to derive the following expressions for $\dot{m}_f$ and $\dot{M}$:

$$\dot{m}_f = \rho_f \beta \bar{X}_f \bar{u} A \quad (5)$$

$$\dot{M} = \bar{\rho} \beta \left(\bar{u} \right)^2 A \quad (6)$$

where the β parameter accounts for the non-uniform velocity and fuel distributions across the spray cross-section, $\bar{X}_f$ and $\bar{u}$ are the turbulent mean cross-sectionally averaged values of the fuel volume fraction and flow velocity, A is the jet cross sectional area, ρ_f is the fuel density (assumed constant) and $\bar{\rho}$ is the turbulent mean cross-sectionally averaged value, which is assumed constant over the entire cross-section. $\bar{\rho}$ is evaluated as follows

$$\bar{\rho} = \rho_f \bar{X}_f + \rho_u (1 - \bar{X}_f) \quad (7)$$

where ρ_u is the density of the unburned gas (made up of air, residual gas and EGR, i.e., exhaust gas recirculation) that surrounds the spray.

$\bar{X}_f$ and $\bar{u}$ are evaluated at each time step and for each control volume as shown in [6]. Finally, the turbulent mean cross-sectionally averaged value of the equivalence ratio, i.e. $\bar{\phi}$, (which is the most important quantity used in the multizone combustion model) is calculated by means of the following equation:

$$\bar{\phi} = \frac{\bar{X}_f \rho_f}{(1 - \bar{X}_f) \rho_u} \left(\frac{m_u}{m_f} \right)_{st} \quad (8)$$

where $\left(\frac{m_u}{m_f} \right)_{st} = \alpha_{st}^u$ is the stoichiometric unburned gas-to-fuel ratio, which depends on the oxygen concentration of the unburned gases, and which is a function of the EGR rate. The boundary condition for Eqs. (1), (2) is the fuel velocity at the nozzle exit, which is derived from the measured injection rate and nozzle hole diameter.

The spreading angle θ of the 1D spray model is usually correlated to the ambient gas-to-injected fuel density ratio [13], but, in this study, it will be taken as a model calibration parameter, and compared with the measured one. In particular, the spreading angle will be tuned in order to match the measured spray penetration, following the procedure reported in [7].

Implementation of the 1D Spray Model in the Multizone Combustion Model

The control volumes ' i ' adopted in the 1D spray model were not used directly as zones in the multizone thermodynamic combustion model, in order to avoid an excessively long computational time. As a consequence, the spray was discretized at each time instant in a user-defined number of mixture zones, which were identified in order to split the total injected fuel mass into equal portions. The procedure is graphically and qualitatively illustrated in Fig. 1.

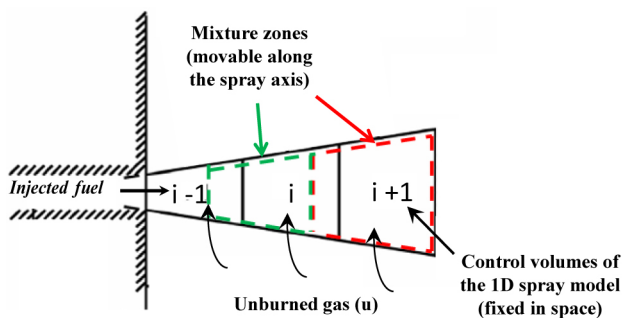


Figure 1. Scheme of the conical spray region, of the 1D spray model control volumes and of the mixture zones used in the combustion model.

Figure 1 reports a schematic of the conic spray region. The control volumes used in the 1D spray model are indicated with the indexes ' $i-1$ ', ' i ', ' $i+1$ ' and bordered with solid black lines. These volumes are fixed in space, and subject to mass and momentum transfer at the boundaries according to Eqs. (1), (2) (Eulerian control volumes). Basically, a fuel parcel is generated by the model at each time step during the injection event. Each parcel penetrates the combustion chamber and progressively mixes with the surrounding unburned gas, thus generating a mixture zone. From a geometrical point of view, each mixture zone can be considered as a slice (bordered with colored dashed lines in Fig. 1) of the conic spray region. The first injected fuel parcel in Fig. 1 is included in the mixture zone bordered by red, which is located at the end of the spray. Although the control volumes remain fixed in space, the mixture zone progressively advances along the spray axis, and occupies different control volumes at different time instants. The fuel parcels that are injected later on are assumed to be located in the portions of the conic region which are progressively closer to the injector nozzle tip (Fig. 1 qualitatively reports the green border of the second mixture zone). With this approach, each mixture zone could occupy more than one control volume of the 1D spray model.

The spray penetration is obtained at each time instant by identifying the last control volume in which the spray velocity $\bar{u}$ is different from zero. The average equivalence ratio of each mixture zone can then be estimated at each time instant on the basis of the solution of the 1D spray model (in particular, from the values of $\bar{X}_f$ related to the involved control volumes), so that the equivalence ratio time history of each mixture zone is obtained as a function of time.

Oxidation is assumed to start at the end of the spray, after the onset of combustion, and to progressively involve the mixture zones closest to the injector tip. This assumption derives from previous investigations carried out by the authors, in which the autoignition time of the different mixture zones was evaluated on the basis of ignition delay correlations such as those reported in [5]. It was found that, in general, the first zones to ignite are those located at the spray tip, and autoignition gradually involves the zones closer to the injector tip. The oxidation rate is derived from the measured in-cylinder pressure time history, as the approach is of a diagnostic type.

Gas Entrainment Correction

The gas entrainment rate derived from the 1D spray has been corrected in order to take into account that the entrainment rate in a real engine is slowed-down by the EGR rate and by the burned gases derived from combustion, following the procedure illustrated in [3]. In particular, the λ increment $d\lambda_j$ of each mixture parcel j was corrected as follows [10]:

$$d\lambda_j = (d\lambda_j)_{1D} \left[1 - \frac{m_{f,burned} (1 + \alpha_{st}^u)}{m^*} \right] \quad (9)$$

where $m_{f,burned}$ is the burned fuel mass, m^* is the total in-chamber mass, and $(d\lambda_j)_{1D}$ is the λ variation estimated by the 1D spray model.

Multizone Combustion Diagnostic Model

Combustion Conceptual Schemes

The conceptual schemes of combustion used in the model depend on the air-to-fuel ratio distribution in the mixture zones at SOC (start of combustion). Three cases, which are summarized hereafter, were considered in the proposed model (see [3]).

Case 1. The mixture zones are lean/stoichiometric at SOC: in this case, the fuel chemical energy can be released completely during the premixed burning.

Case 2. The whole air-to-fuel mixture ratio is rich at SOC: in this case, the fuel chemical energy can only be released completely through the two-stage premixed-diffusive conceptual scheme described by Dec in [9].

Case 3. This is an intermediate case between cases 1 and 2. There are in fact some cases in which the first fuel parcels, which are located at the end of the spray (e.g., red zone in Fig. 1), burn with a rich air-to-fuel ratio (therefore following the Dec conceptual scheme), whereas the parcels that are injected later on (e.g., green zone in Fig. 1) have sufficient time to reach stoichiometric/lean conditions before oxidation, without soot formation.

Model Equations

The model is based on the application of the energy and mass conservation laws to the different zones identified in the combustion chamber.

An unburned gas zone, made up of a mixture of trapped fresh air, EGR and residual gas is generated from IVC (Intake Valve Closure) onwards. This zone is progressively compressed by the piston, and is characterized by a constant mass, equal to the total trapped mass, until SOI (start of injection). The total trapped mass is calculated as follows:

$$m_{trap}^* = m_a^* + m_{res}^* + m_{EGR}^* \quad (10)$$

where the asterisk denotes a constant quantity in time.

The air mass is calculated by multiplying the experimentally-evaluated injected fuel mass by the air-to-fuel ratio α , which is in turn evaluated on the basis of the measured emissions with the procedure explained in [14]. The EGR mass is calculated on the basis of the experimental EGR rate, which can be calculated by means of a procedure that is based on the measurement of the intake manifold CO_2 concentration, and which is also explained in [14].

A user-defined number M_j of mixture zones (m) is progressively generated (see Fig. 1) after the SOI for the generic injection shot j ($1 \leq j \leq J$), where J is the total number of injection shots; these mixture zones are constituted by vaporized fuel and unburned gas, where the unburned gas entrainment is derived from the 1D spray model solution.

A premixed burned gas zone (bp) is generated at the SOPC (start of premixed combustion), which progressively consumes all the generated mixture zones.

The SOPC is calculated for the first injection shot on the basis of the application of the energy conservation law to the whole combustion chamber content. The start of combustion is represented by the first energy-fraction release, and should therefore be detected when the cylinder pressure begins to differentiate from the pressure time-history in the absence of combustion.

In the cases in which the oxidation of the fuel of the second injection shot begins after the complete consumption of the mixture zones of the first injection shot (i.e., for relatively large dwell times between two consecutive shots), the model identifies the actual start of the oxidation of the second injection from the analysis of the pressure time history. Instead, in the cases in which the oxidation of two consecutive injection shots overlaps (i.e., for short dwell times), the fuel parcels derived from the first and the second injection pulses are assigned to the same mixture zone, whose air-to-fuel ratio is evaluated according to the 1D spray model. In this case, the model identifies the SOPC of the first injection shot, and the oxidation proceeds according to the experimentally-derived heat release rate, involving the required fuel mass from the mixture zone.

With reference to the start of diffusive combustion (SODC), it should be pointed out that different combustion schemes can occur, as mentioned in the previous section.

In case 1, the mixture zones are stoichiometric/lean at the start of combustion, thus the fuel chemical energy can be released completely during the premixed burning and no SODC is detected. In cases 2-3, the mixture zones at the start of combustion are rich, therefore a rich premixed burned gas zone (bp) is generated at the SOPC, and it progressively consumes the rich mixture zones. After the onset of diffusive combustion (SODC), N_j diffusive burned gas zones (bd) are progressively generated to complete the oxidation of the rich premixed combustion products. As far as the identification of the SODC is concerned, it was shown in [15] that the diffusive combustion at the jet periphery starts very early during the premixed peak, about 2-3 deg after the SOPC. These values have been used as a reference to set the SODC.

A different set of zones has been generated separately for each injection shot. When the mixture zones of the previous injection shot are consumed completely, the mixture zones of the next injection shot start oxidizing. The oxidation process is governed by the experimental pressure signal, therefore no oxidation model is required for combustion diagnostic purposes.

The multizone approach stems from application of the mass and energy conservation laws to each zone, along with the perfect gas equation for each gaseous zone. The energy conservation of each zone in the time interval ($dt=dCA/\omega$) can be written as follows:

$$\delta Q + Vdp = dH + \left| \dot{H}_{out} \right| dt - \left| \dot{H}_{in} \right| dt$$

where Q denotes the heat transfer with the walls, V the volume of the zone, p the pressure and H the enthalpy.

The equations related to the Dec conceptual scheme (i.e., case 2) are reported here for the sake of brevity. However, the reader can refer to [3] for the whole set of equations, including case 1 and case 3. The combustion conceptual scheme for case 2 is reported in Fig. 2.

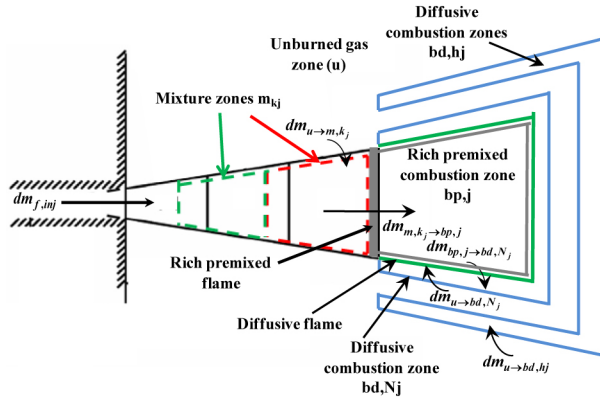


Figure 2. Combustion conceptual scheme for case 2 [3].

The following energy equations hold for the different zones:

$$\delta Q_u + V_u dp = m_u dh_u \quad (12)$$

$$\begin{aligned} \delta Q_{m,k_j} + V_{m,k_j} dp &= m_{m,k_j} dh_{m,k_j} + dm_{f,inj} (h_{m,k_j} - h_{f,i}) + \\ dm_{u \rightarrow m,k_j} (h_{m,k_j} - h_u) \quad (1 \leq k_j \leq M_j) \quad (1 \leq j \leq J) \end{aligned} \quad (13)$$

$$\begin{aligned} \delta Q_{bp,j} + V_{bp,j} dp &= m_{bp,j} dh_{bp,j} + \\ + \sum_{k_j=1}^{M_j} dm_{m,k_j \rightarrow bp,j} (h_{bp,j} - h_{m,k_j}) \quad (1 \leq j \leq J) \end{aligned} \quad (14)$$

$$\begin{aligned} \delta Q_{bd,n_j} + V_{bd,n_j} dp &= m_{bd,n_j} dh_{bd,n_j} + dm_{u \rightarrow bd,n_j} (h_{bd,n_j} - h_u) \\ (1 \leq n_j < N_j) \quad (1 \leq j \leq J) \end{aligned} \quad (15)$$

$$\begin{aligned} \delta Q_{bd,N_j} + V_{bd,N_j} dp &= m_{bd,N_j} dh_{bd,N_j} + \\ + dm_{bp,j \rightarrow bd,N_j} (h_{bd,N_j} - h_{bp,j}) + \\ + dm_{u \rightarrow bd,N_j} (h_{bd,N_j} - h_u) \quad (1 \leq j \leq J) \end{aligned} \quad (16)$$

The mass increment of a specific zone is indicated by adding the index of that zone to dm , whereas the mass transfer between adjacent zones is shown with a subscript in dm , which consists of an arrow between the zone indexes. dm is positive if the mass transfer occurs in the arrow direction.

The enthalpy convection terms on the right hand side of Eqs. (13), (14), (15), (16) are related to the mass transfer between adjacent zones. In other words, the mixture zones are fed with mass from the injected fuel and the unburned gas zone, and deliver mass to the premixed burned gas zones as a consequence of the premixed combustion. The premixed burned gas zones receive mass from the mixture zones and give mass to the diffusive burned gas zones after the onset of diffusive combustion, so that the rich premixed combustion products complete their oxidation. The diffusive burned gas zones N_j receive mass from the premixed burned gas zones j and from the unburned gas zone, in order to reach stoichiometric conditions. The post-combustion diffusive burned gas zones n_j ($1 \leq n_j < N_j$) are progressively diluted with the unburned gas, where $dm_{u \rightarrow bd,n_j}$ is the dilution term.

The mass conservation equations can be written as follows:

$$dm_u = - \sum_{j=1}^J \sum_{k_j=1}^{M_j} dm_{u \rightarrow m,k_j} - \sum_{j=1}^J \sum_{n_j=1}^{N_j} dm_{u \rightarrow bd,n_j} \quad (17)$$

$$\begin{aligned} dm_{m,k_j} &= dm_{f,inj} + dm_{u \rightarrow m,k_j} - dm_{m,k_j \rightarrow bp,j} \\ (1 \leq k_j \leq M_j) \quad (1 \leq j \leq J) \end{aligned} \quad (18)$$

$$\begin{aligned} dm_{bp,j} &= \sum_{k_j=1}^{M_j} dm_{m,k_j \rightarrow bp,j} - dm_{bp,j \rightarrow bd,N_j} \\ (1 \leq j \leq J) \end{aligned} \quad (19)$$

$$\begin{aligned} dm_{bd,n_j} &= dm_{u \rightarrow bd,n_j} \\ (1 \leq n_j < N_j) \quad (1 \leq j \leq J) \end{aligned} \quad (20)$$

$$\begin{aligned} dm_{bd,N_j} &= dm_{bp,j \rightarrow bd,N_j} + dm_{u \rightarrow bd,N_j} \\ (1 \leq j \leq J) \end{aligned} \quad (21)$$

Equation system (12, 13, 14, 15, 16, 17, 18, 19, 20, 21) has to be coupled to the relation obtained by making the sum of the different zone volumes equal to the instantaneous cylinder volume V :

$$\begin{aligned} pV &= m_u R_u T_u + \sum_{j=1}^J \sum_{k_j=1}^{M_j} m_{m,k_j} R_{m,k_j} T_{m,k_j} + \\ + \sum_{j=1}^J m_{bp,j} R_{bp,j} T_{bp,j} + \sum_{j=1}^J \sum_{n_j=1}^{N_j} m_{bd,n_j} R_{bd,n_j} T_{bd,n_j} \end{aligned} \quad (22)$$

Equation (22) is an explicit function of pressure p , which is acquired experimentally, as the approach is of a diagnostic type.

Only Eqs. (12), (13), (14) and (17), (18), (19) are considered for the combustion scheme labeled 'case 1'.

As far as the case 3 combustion scheme is concerned, the reader can refer to [3] for the detailed set of equations.

The thermodynamic properties of each species are determined through the JANAF tables, by carrying out a multiple species equilibrium composition calculation for the burned gas zones, in which dissociation is taken into account. The model is also capable of taking into account the flexible composition of the fuel and the intake air humidity.

The diffusive burned gas zones can be considered to be either mixing or non-mixing with the surrounding unburned gas after combustion. In this paper, the mixing effect is taken into account according to the approach proposed in [16, 17]:

$$\lambda_{bd,n_j} = \lambda_c + (\lambda - \lambda_c) \left\{ 1 - \exp \left[-C \left(\frac{CA - CA_0}{CA_{EVO} - CA} \right)^M \right] \right\} \quad (23)$$

where λ_{bd,n_j} is the relative air/fuel ratio of the diffusive burned gas zone bd,n_j , λ_c is the diffusive combustion relative air/fuel ratio, λ is the global in-chamber relative air/fuel ratio, and CA , CA_0 and CA_{EVO} are the generic crank angle, the crank angle at which the zone is generated and the EVO (exhaust valve opening) crank angle, respectively. Coefficient C was set to 6.908, as suggested in [17], while coefficients λ_c and M were treated as tuning coefficients [4].

It should be pointed out that Eq. (23) is used to model the relative air/fuel ratio of the diffusive burned gas zones, which is related to the soot oxidation process to a great extent. The soot formation rate, instead, depends on the spray equivalence ratio during premixed combustion, which is evaluated by means of the 1D spray model.

The differentials of the diffusive, premixed and global released chemical energy associated with injection shot 'j' can be evaluated as follows:

$$dQ_{ch,bd,n_j} = dm_{bp,j \rightarrow bd,n_j} (h_{bp,j} - h_{bd,n_j}) + dm_{u \rightarrow bd,n_j} (h_u - h_{bd,n_j}) \quad (24)$$

$$dQ_{ch,bp,j} = \sum_{k_j=1}^{M_j} dm_{m,k_j \rightarrow bp,j} (h_{m,k_j} - h_{bp,j}) \quad (25)$$

$$dQ_{ch,j} = dQ_{ch,bd,j} + dQ_{ch,bp,j} \quad (26)$$

The heat exchanged with the walls by each zone in the time interval dt is evaluated, in Eqs. (12), (13), (14), (15), (16), taking into account a convective term and a radiative term, where the latter is due to the presence of soot particles, so that:

$$\delta Q = \left[h A (T - T_w) + k_{rad} A (T^4 - T_w^4) \right] dt \quad (27)$$

The convective coefficient h for each zone is calculated according to the Woschni correlation [18, 19, 20], where A is the heat transfer surface area of the zone, which is considered to be a fraction of the total surface area of the combustion chamber and equal to the mass fraction of the zone, and k_{rad} is a radiative heat transfer coefficient. The heat transfer coefficients are tuned so that the computed and experimental combustion efficiencies are equal. To this end, the approach that was presented in [1, 2, 3] is followed.

Soot Formation Model

Soot formation is modeled by means of an expression that directly accounts for the average value of ϕ during combustion, according to a similar approach to the one presented in [10]:

$$\frac{dm_{sf}}{dt} (t + \tau_{d,sf}) = C_{soot} \cdot \sqrt{(\phi(t) - 2)} \cdot \sqrt{p(t)} \cdot K_T(t) \cdot m_{f,v}(t) \quad (28)$$

where $(\phi-2)$ is the soot formation dependence on the equivalence ratio, p is the pressure, $m_{f,v}$ is the evaporated fuel mass, and C_{soot} is a calibration constant which was set to 0.05 according to [10]. Equation (28) is inspired by Kaario et al [21], who in turn were inspired by Kitamura et al [8]. Unlike the equation proposed in [10], a parameter related to the delay in soot formation, i.e., $\tau_{d,sf}$ had to be introduced in order to match the experimental and predicted soot formation trends. This is coherent with the results of the previous study reported in [4].

In Eq. (28), K_T is a temperature term, which is expressed as follows:

$$K_T = \left[1 - e^{-7 \left(\frac{T-1300}{1800-1300} \right)^3} \right], \quad T < 1800K \quad (29)$$

$$K_T = \left[e^{-7 \left(\frac{T-1800}{2300-1800} \right)^3} \right], \quad T \geq 1800K \quad (30)$$

The soot mass oxidation rate is modeled by the Nagle and Strickland-Constable empirical formula [5]:

$$\frac{dm_{so}}{dt} = \frac{6 \cdot m_s}{\rho_s D_s} M_C R_{tot} \quad (31)$$

where m_s is the soot mass, ρ_s the soot density, D_s the mean soot diameter, M_C the carbon atomic mass and R_{tot} the surface mass oxidation rate:

$$R_{tot} = \frac{k_A p_{O_2}}{1 + k_Z p_{O_2}} x_A + k_B p_{O_2} (1 - x_A) \quad (32)$$