

Assessment of a New Quasi-Dimensional Multizone Combustion Model for the Spray and Soot Formation Analysis in an Optical Single Cylinder Diesel Engine

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ABSTRACT

An innovative quasi-dimensional multizone combustion model for the spray formation, combustion and emission formation analysis in DI diesel engines was assessed and applied to an optical single cylinder engine.

The model, which has been recently presented by the authors, integrates a predictive non stationary 1D spray model developed by the Sandia National Laboratory, with a diagnostic multizone thermodynamic model.

The 1D spray model is capable of predicting the equivalence ratio of the fuel during the mixing process, as well as the spray penetration.

The multizone approach is based on the application of the mass and energy conservation laws to several homogeneous zones identified in the combustion chamber. A specific submodel is also implemented to simulate the dilution of the burned gases.

Soot formation is modeled by an expression which derives from Kitamura et al.'s results, in which an explicit dependence on the local equivalence ratio is considered.

The model was used to analyze low load (BMEP = 2 bar at 1500 rpm) and medium load (BMEP = 5 bar at 2000 rpm) operating conditions in an optical single cylinder engine sharing the combustion system configuration of the 2.0L Euro5 GM diesel engine for passenger car application. The images obtained by a CCD camera were used to derive statistically averaged values of the spray tip penetration and of the dispersion angle. The soot concentration was also calculated by means of the two-colour pyrometry method. These experimental data were used for the multizone model assessment.

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INTRODUCTION

The engine calibration activity at the test bench requires the analysis of several calibration parameters and of their effects on the main target functions to be optimized, such as the emissions, the fuel consumption and the combustion noise [1]. The interpretation of the cause and effect relationships is not obvious and immediate to be understood from the raw experimental datasets. To this end, zero-dimensional and quasi-dimensional combustion models can be of fundamental importance in order to add further information to the experimental results.

In this context, an innovative quasi-dimensional multizone diagnostic combustion model [2, 3] has been developed by the authors for the analysis of the spray formation, combustion processes and emission formation in direct injection (DI) diesel engines. The model is a refinement of a previous version presented in [4]. In particular, the main novelty consists of the integration of a predictive 1D spray model developed by the Sandia National Laboratory [5, 6] with a multizone diagnostic combustion model.

Basically, the spray model is capable of evaluating the spray penetration and the average equivalence ratio of the

injected fuel parcels as a function of the spray axial distance and time.

The combustion process is modeled by a multizone 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 the energy and mass conservation principles are applied. Several combustion conceptual schemes are adopted starting from the Dec one [7], and extending it also for highly premixed combustion cases [2]. Premixed and diffusive contributions to the heat release rate are taken into account.

The modeling of the spray formation is fundamental for an accurate evaluation of the soot formation process, which mainly depends on the local equivalence ratio dynamics during the fuel/charge mixing and at the early stages of combustion [8].

Main model outcomes are also the temperature and mass evolutions of the different zones, along with their chemical composition. These quantities allows the implementation of specific submodels for the calculation of NO, CO, soot and THC [2, 3].

The integration of a combustion diagnostic multizone approach with a non-stationary 1D spray model is innovative.

As a matter of fact, similar approaches have already been presented in the literature, e.g. those reported in [9-10], but they include a free, fully developed, quasi-steady fuel spray model, such as the one presented in [11].

Other studies have been recently conducted in ([12-13]) about the modeling of the liquid spray penetration and of a reacting diesel jet respectively, considering a non-steady jet model. The latter study is focused on the modeling of mixing-controlled reacting diesel jets, whereas the approach proposed by the authors in this paper includes a detailed thermodynamic model which considers premixed and diffusive combustion phases and different conceptual schemes.

The use of a non-stationary model to simulate the spray dynamics is of crucial importance, because it allows the real injection rate profile used in the engine to be implemented as model input. It therefore allows the effects of the shape of the injection rate on the equivalence ratio distribution of the spray to be taken into account, as well as "entrainment wave" effects as those reported in [5].

Another novelty of the proposed model concerns the implementation of a post-combustion mixing and cooling submodel in order to take into account the dilution of the burned gases produced from diffusive combustion. The latter has a great impact on the oxidation process of the in-cylinder pollutant emissions, and especially on soot.

In the present paper, the model has been applied and assessed on a single-cylinder engine. The images obtained by a CCD camera were used to derive statistically averaged values of the spray tip penetration and of the dispersion angle at low load (BMEP = 2 bar at 1500 rpm) and medium load (BMEP = 5 bar at 2000 rpm) operating conditions. The soot

concentration was also calculated by means of the two-colour pyrometry method.

These experimental data were found to be fundamental for the assessment of the multizone model. In particular, the experimental spray penetration and dispersion angles were used for the calibration of the 1D spray model, whereas the experimental soot concentration was found to provide useful information for the calibration of the burned gas dilution submodel.

MODEL DESCRIPTION

1d Spray Model

For a complete description of the 1D spray model the reader should refer to [5, 6].

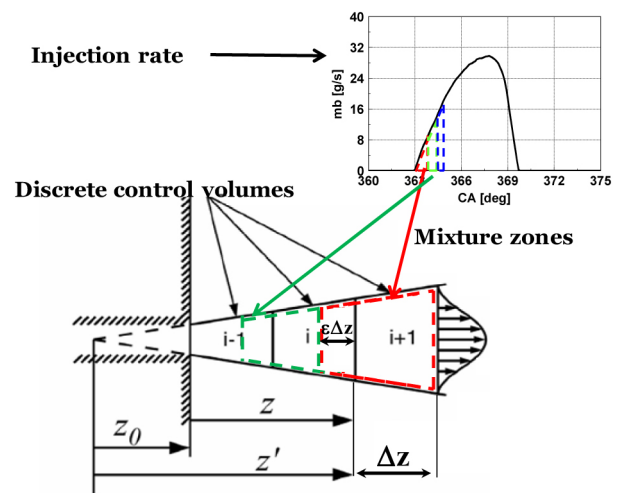


Figure 1. Schematic of the spray conic region in which the discrete control volumes and the mixture zones are reported, along with an injection rate example (top) ([2]).

In what follows, the quantities related to the liquid fuel are denoted with the subscript 'f', and those related to the in-cylinder fresh charge are denoted with the subscript 'u' (unburned gas). The spray is considered as a conic-shaped region with a spreading angle θ (Fig. 1), which is discretized into several control volumes i , for which the transient transport equations for fuel mass m_f and axial momentum M are written as follows:

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

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

By assuming a distribution of the turbulent mean fuel volume fraction $\bar{X}_f$ and of the turbulent mean velocity $\bar{u}$ ([5, 6]), of the type:

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

$$\frac{\bar{u}}{\bar{u}_c} = (1 - \xi^\alpha)^2 \quad (4)$$

the following expressions can be derived for $\dot{m}_f$ and $\dot{M}$:

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

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

where $\bar{\beta} = \frac{6(\alpha+1)(\alpha+2)}{(3\alpha+2)(2\alpha+1)}$.

The β parameter accounts for the non-uniform velocity and fuel distributions across the spray cross-section.

In Eqs. (3, 4), $\xi = r/R$ 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, 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 ($\alpha = 1.5$). $\bar{X}_f$ 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.

Equation (6) was derived under the assumption of a constant density, over the entire cross-section, equal to the turbulent mean cross-sectionally averaged value $\bar{\rho}$:

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

The quantities that are calculated at each time instant in the control volumes are the fuel mass m_f and the total axial momentum M . As a consequence, the turbulent mean cross-sectionally averaged fuel mass fraction and axial velocity are obtained as follows:

$$\bar{X}_f = \frac{m_f / \rho_f}{A \Delta z} \quad (8)$$

$$\bar{u} = \frac{M}{\bar{\rho} A \Delta z} \quad (9)$$

Finally, the turbulent mean cross-sectionally averaged value of the equivalence ratio, i.e. $\bar{\phi}$, is calculated by means of the following equation:

$$\bar{\phi} = \frac{\bar{X}_f \rho_f}{(1 - \bar{X}_f) \rho_u} \left(\frac{m_u}{m_f} \right)_{st} \quad (10)$$

The experimental injection rate is assumed to be known, and it is necessary to calculate the fuel velocity at the nozzle exit, which is the boundary condition.

The spreading angle θ of the 1D spray model is usually correlated to the ambient gas-to-injected fuel density ratio ([14]).

In the present paper, a sensitivity study has been carried out, in order to investigate its effects on the spray penetration and equivalence ratio distribution taking into account the available experimental data.

The total number of control volumes ' i ' adopted in the 1D spray model cannot be directly treated as zones in the multizone thermodynamic combustion model, because it is very high and it would lead to an excessive computational time. As a consequence, the spray is discretized at each time instant in a user-defined number of mixture zones, which are identified in order to split the total injected fuel mass into equal portions. The unburned gas entrainment in each mixture zone is calculated by the 1D spray model. Within this approach, each mixture zone could occupy more than one control volume of the 1D spray model.

The procedure is graphically and qualitatively illustrated in Fig. 1. The left part of Fig. 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 (Eulerian control volumes). The right part of Fig. 1 shows a typical injection rate. Basically, a fuel parcel (bordered with colored dashed lines in the upper part of Fig. 1) 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. From a geometrical point of view, each mixture zone can be considered as a slice (bordered with colored dashed lines in the left part of 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 (the left part of Fig. 1 qualitatively reports the green border of the second mixture zone). After injection, the fuel parcels mix and penetrate the spray axis.

If the jet penetration is known at each time instant (corresponding to the last control volume in which the spray velocity $\bar{u}$ is different from zero), the mixture zones can be identified by integrating the fuel concentration in the different control volumes, starting from the jet penetration position and moving towards the injector tip, until the mass of the associated fuel parcel is obtained. A mixture zone can occupy more than one control volume and/or a portion of a control

volume. The average equivalence ratio of each mixture zone can then be estimated at each time instant from the turbulent mean cross-sectionally averaged fuel mass fraction of the involved control volumes (and/or portion of control volumes). This procedure is applied to all the generated mixture zones for all the time instants after the start of injection, so that the equivalence ratio time history of each mixture zone is obtained as a function of time.

After the onset of combustion, oxidation is assumed to start at the end of the spray, and to progressively involve the mixture zones closest to the injector tip. The oxidation rate is derived from the measured in-cylinder pressure time history, being the approach of the diagnostic type.

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 (exhaust gas recirculation) rate and by the burned gases derived from combustion. As shown in [2], the EGR rate effect is taken into account in Eq. (10), in which the term

$\left(\frac{m_u}{m_f}\right)_{st} = \alpha_{st}^u$ is calculated as a function of the EGR rate. In order to account for the in-cylinder burned gas effect, the λ increment $d\lambda_j$ of each mixture parcel j is corrected as follows ([9]):

$$d\lambda_j = (d\lambda_j)_{1D} \left[1 - \frac{m_{f,burned} (1 + \alpha_{st}^u)}{m^*} \right] \quad (11)$$

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 scheme

The conceptual scheme of combustion is influenced by the air-to-fuel ratio distribution in the mixture zone at SOC (start of combustion). For a detailed description of the combustion conceptual schemes, the reader should refer to [2]. Basically, three cases are taken into account.

Case 1. The whole mixture is lean/stoichiometric at SOC: in this case, the fuel chemical energy can be completely released during the premixed burning. A high entrainment rate of the unburned gas in the spray occurs before combustion, due to the high ignition delay, and a stoichiometric/lean premixed combustion occurs. This case generally describes the combustion process for pilot injections and, more in general, for very highly premixed combustion.

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 [7]. All the fuel parcels undergo a rich premixed phase, whose combustion

products complete oxidation in a thin diffusion flame at the jet periphery.

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

Model equations

The multizone diagnostic 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, which is progressively compressed by the piston movement. The EGR rate was calculated by means of a procedure that was developed by the authors and which is based on the measurement of the intake manifold CO_2 concentration ([15]).

After the SOI, a user-defined number M_j of mixture zones (m) is progressively generated 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.

In the case of multiple injections, the combustion of the pilot shots, considering the related high ignition delay, is assumed to occur in fully premixed conditions. Thus, 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 injected pilot shot according to the procedure detailed in [2, 3, 4], which is based on 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, thus, should be detected when the cylinder pressure begins to differentiate from the pressure time-history in the absence of combustion. When the oxidation of the fuel of the second injection shot begins after the complete consumption of the mixture zones of the first injection (i.e., 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. When the oxidation of two consecutive injection shots overlaps (i.e., short dwell times), the fuel parcels deriving from the first and the second injection pulses are assigned to the same mixture zone, whose air-to-fuel ratio is evaluated according to 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, combustion occurs in fully premixed stoichiometric/lean conditions, therefore no SODC is detected.

In cases 2-3, a rich premixed burned gas zone (bp) is generated at the SOPC, and it progressively consumes the 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 [16] 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 for the setting of the SODC.

A different set of zones is generated separately for each injection shot. When the mixture zones of the previous injection shot are completely consumed, 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 the applications 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:

$$\delta Q + V dp = dH + \left| \dot{H}_{out} \right| dt - \left| \dot{H}_{in} \right| dt \quad (12)$$

By modeling the combustion process with the Dec combustion scheme (case 2), according to which all mixture parcels burn in rich conditions and complete their oxidation in the stoichiometric diffusive zones, and introducing the previously defined indexes, the following energy equations hold for the different zones:

$$\delta Q_u + V_u dp = m_u dh_u \quad (13)$$

$$\begin{aligned} \delta Q_{m,k_j} + V_{m,k_j} dp &= m_{m,k_j} dh_{m,k_j} + dm_{f,inj} (h_{m,k_j} - h_{f,l}) + \\ &dm_{u \rightarrow m,k_j} (h_{m,k_j} - h_u) \quad (1 \leq k_j \leq M_j) ; (1 \leq j \leq J) \end{aligned} \quad (14)$$

$$\begin{aligned} \delta Q_{bp,j} + V_{bp,j} dp &= m_{bp,j} dh_{bp,j} + \\ &+ \sum_{k_j=1}^{M_j} dm_{m,k_j \rightarrow bp,j} (h_{bp,j} - h_{m,k_j}) \quad (1 \leq j \leq J) \end{aligned} \quad (15)$$

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

$$\begin{aligned} \delta Q_{bd,N_j} + V_{bd,N_j} dp &= m_{bd,N_j} dh_{bd,N_j} + \\ &+ dm_{bp,j \rightarrow bd,N_j} (h_{bd,N_j} - h_{bp,j}) + \\ &+ dm_{u \rightarrow bd,N_j} (h_{bd,N_j} - h_u) \quad (1 \leq j \leq J) \end{aligned} \quad (17)$$

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. (14, 15, 16, 17) are related to the mass transfer between adjacent zones. More in detail, 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 products of rich premixed combustion 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, being $dm_{u \rightarrow bd,n_j}$ the dilution term.

The mass conservation equations can be written as follows:

$$dm_u = - \sum_{j=1}^J \sum_{k_j=1}^{M_j} dm_{u \rightarrow m,k_j} - \sum_{j=1}^J \sum_{n_j=1}^{N_j} dm_{u \rightarrow bd,n_j} \quad (18)$$

$$\begin{aligned} dm_{m,k_j} &= dm_{f,inj} + dm_{u \rightarrow m,k_j} - dm_{m,k_j \rightarrow bp,j} \\ &(1 \leq k_j \leq M_j) ; (1 \leq j \leq J) \end{aligned} \quad (19)$$

$$dm_{bp,j} = \sum_{k_j=1}^{M_j} dm_{m,k_j \rightarrow bp,j} - dm_{bp,j \rightarrow bd,N_j} \quad (1 \leq j \leq J) \quad (20)$$

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

$$\begin{aligned} dm_{bd,N_j} &= dm_{bp,j \rightarrow bd,N_j} + dm_{u \rightarrow bd,N_j} \\ &(1 \leq j \leq J) \end{aligned} \quad (22)$$

Equation system (13, 14, 15, 16, 17, 18, 19, 20, 21, 22) has to be coupled to the relation obtained by making the sum

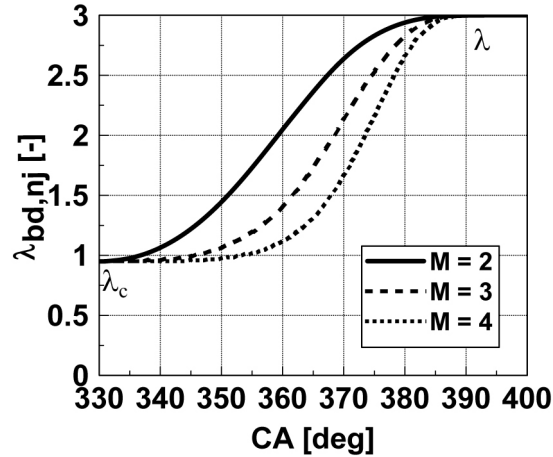


Figure 2. Plot of $\lambda_{bd,nj}$ vs. CA according to Eq. (24), for three different values of M ($C=6.908$).

of the different zone volumes equal to the instantaneous cylinder volume V :

$$pV = m_u R_u T_u + \sum_{j=1}^J \sum_{k_j=1}^{M_j} m_{m,k_j} R_{m,k_j} T_{m,k_j} + \sum_{j=1}^J m_{bp,j} R_{bp,j} T_{bp,j} + \sum_{j=1}^J \sum_{n_j=1}^{N_j} m_{bd,n_j} R_{bd,n_j} T_{bd,n_j} \quad (23)$$

Equation (23) is an explicit function of the pressure p , which is acquired experimentally, being the approach of the diagnostic type.

Only Eqs. (13, 14, 15) and (18, 19, 20) are considered for the combustion scheme labeled as 'case 1'.

As far as case 3 combustion scheme is concerned, the reader can refer to [2] for the detailed 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 fuel flexible composition and intake air humidity.

Post combustion mixing and cooling model

The diffusive burned gas zones can be considered 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 [17, 18]:

$$\lambda_{bd,n_j} = \lambda_c + (\lambda - \lambda_c) \left\{ 1 - \exp \left[-C \left(\frac{CA - CA_0}{CA_{EVO} - CA} \right)^M \right] \right\} \quad (24)$$

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 in-chamber global relative air/fuel ratio, CA, CA_0 and CA_{EVO} are the generic crank angle, the crank angle at which the zone is generated and EVO (exhaust valve

opening) crank angle, respectively. In accordance with [18], coefficient C was set to 6.908, whereas a sensitivity analysis was carried out on the coefficients λ_c and M , in order to match the predicted and experimentally-derived in-cylinder soot trends. Figure 2 shows the shape of Eq. (24) for three different values of M , being $C=6.908$. It has to be pointed out that Eq. (24) is used to model the relative air/fuel ratio of the diffusive burned gas zones, which is strongly related to the soot oxidation process. The soot formation rate, instead, depends on the spray equivalence ratio during the premixed combustion, which is evaluated by the 1D spray model

Chemical energy release

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

$$dQ_{ch,bd,N_j} = dm_{bp,j \rightarrow bd,N_j} (h_{bp,j} - h_{bd,N_j}) + dm_{u \rightarrow bd,N_j} (h_u - h_{bd,N_j}) \quad (25)$$

$$dQ_{ch,bp,j} = \sum_{k_j=1}^{M_j} dm_{m,k_j \rightarrow bp,j} (h_{m,k_j} - h_{bp,j}) \quad (26)$$

$$dQ_{ch,j} = dQ_{ch,bd,j} + dQ_{ch,bp,j} \quad (27)$$

Heat Transfer and Calibration Procedure

The heat exchanged with the walls by each zone in the time interval dt , is evaluated in Eqs. (13, 14, 15, 16, 17), not only by means of a convective term, but also with a radiative contribution, due to the presence of soot particles ([6]), so that:

$$\delta Q = \left[h A (T - T_w) + k_{rad} A (T^4 - T_w^4) \right] dt \quad (28)$$

The convective coefficient h for each zone is calculated according to the Woschni correlation [19, 20, 21], where τ is