

Analysis of Combustion and Emissions in a EURO V Diesel Engine by Means of a Refined Quasi-Dimensional Multizone Diagnostic Model

Roberto Finesso and Ezio Spessa
Politecnico di Torino

ABSTRACT

A quasi dimensional multizone combustion model, that was previously developed by the authors, has been refined and applied for the analysis of combustion and emission formation in a EURO V diesel engine equipped with a piezo indirect-acting injection system.

The model is based on the integration of the predictive non stationary variable-profile 1D spray model recently presented by Musculus and Kattke, with a diagnostic multizone thermodynamic model specifically developed by the authors.

The multizone approach has been developed starting from the Dec conceptual scheme, and is based on the identification of several homogeneous zones in the combustion chamber, to which mass and energy conservation laws have been applied: an unburned gas zone, made up of air, EGR (Exhaust Gas Recirculation) and residual gas, several fuel/unburned gas mixture zones, premixed combustion burned gas zones and diffusive combustion burned gas zones. The fuel parcels first undergo a premixed combustion phase; if the latter occurs in rich conditions, the incomplete combustion products are oxidized by a stoichiometric diffusive flame at the periphery of the jet.

The 1D spray model is capable of calculating the mixing process dynamics of the fuel parcels with the unburned gas, starting from the experimentally-derived injection rate, and of evaluating the equivalence of the mixture zones as a function of time. The oxidation rate of the mixture zones is derived from the experimental pressure trace, which is used as an input quantity for the model, since the approach is of the diagnostic type.

The main model outcomes are the in-chamber mass and temperature evolutions of the different zones, which are used for the subsequent implementation of the submodels that are capable of evaluating the formation of NO_x (Nitrogen Oxides), CO (Carbon Monoxide), soot and THC (Total Unburned Hydrocarbons).

In the present paper, the quasi-dimensional model has been refined by means of the implementation and assessment of a specific submodel which is used to evaluate the post-combustion mixing dynamics of the burned gases with the surrounding unburned gas. A detailed comparison between the results obtained with the original and the refined approaches has been carried out, and the main effects on the pollutant formation submodels have been analyzed in great detail. The complete model, including the post-combustion dilution of the burned gas, was then applied to investigate the effects of different injection calibration parameters, such as rail pressure, number of injection shots, and DT (dwell-time) between the pilot and main injections, on combustion and emissions, with particular reference to the interaction between the spray dynamics and the soot formation process.

CITATION: Finesso, R. and Spessa, E., "Analysis of Combustion and Emissions in a EURO V Diesel Engine by Means of a Refined Quasi-Dimensional Multizone Diagnostic Model," *SAE Int. J. Engines* 5(3):2012, doi:10.4271/2012-01-1066.

INTRODUCTION

The calibration activity of diesel engines at the test bench requires the investigation of the effects of a large number of engine operating variables on the combustion process and pollutant emission levels, for different engine operating conditions. To this end, DoE (Design of Experiment)

techniques have demonstrated to be valid methodologies ([1]), considering that full factorial approaches are not viable.

The DoE methodology can be summarized as follows. The first step involves the definition of the response variables and the input parameters that mainly control the system response. The main response variables are FC (fuel consumption), CN (combustion noise) and the main pollutant



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specific emissions, such as NO_x , CO, soot and THC. The input parameters that control the system response are the fuel injected quantities, the DT between multiple injections, the main injection timing, the rail pressure, the swirl level and the trapped air mass. A mathematical model of the system response, which is usually a polynomial function, is then defined. Then, an experimental plan, made up of variation lists for the different input variables, is set up and carried out in order to identify the model coefficients for the different response variables. The total number of experimental tests is selected on the basis of a trade-off between the experimental effort and the required model predictive capability. Finally, target functions, which account for the above-mentioned response variables, are introduced with weight factors that depend on the target of the optimization. Different sets of engine calibration parameters can be identified, depending on the specific target function that has to be minimized.

It is obvious that such a mathematical procedure does not allow a critical interpretation of the cause and effect relationships between the input parameters and the response variables. To this end, the quasi-dimensional multizone premixed-diffusion diagnostic combustion model presented in [2], and refined in this paper, can be of fundamental importance in order to add further information to the experimental results.

The proposed approach is based on the integration of a predictive 1D nonstationary spray model, which has recently been presented by Musculus et al. ([3, 4]), with a multizone zero-dimensional combustion model that was previously developed by the authors in ([5]), starting from the Dec conceptual scheme ([6]). 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 ([7]). As the approach is of a diagnostic type, the in-cylinder experimental pressure trace is acquired and used as model input to evaluate the fuel burning rate, at an equivalence ratio that is calculated by the 1D spray model at each time instant.

Similar approaches have already been presented in the literature, e.g. those reported in [8] by Westlund et al. and in [9] by Seykens et al. A predictive combustion model is reported in [8]. In this model, the mixing process of the different fuel parcels is calculated adopting a one-dimensional model for a free, fully developed, quasi-steady fuel spray, such as the one presented by Naber and Siebers in [10]. This model is corrected by taking into account the effect of the burned gas and EGR gases. A diagnostic combustion model is presented in [9]. This model is based on a two-phase premixed-diffusive Dec combustion scheme, like the one presented in this paper. In [9], the ambient gas/fuel packages are assumed to mix with the surrounding gas in the same way as the Naber and Siebers fully-developed jet ([10]).

The main novelty of the approach proposed by the authors in [2] and which has been further refined in this paper

through the introduction of a dilution burned gas submodel, is that: it couples the multizone diagnostic combustion approach ([5]), which was derived from the two-stage premixed-diffusive Dec conceptual scheme, with the nonstationary variable profile 1D spray model reported in ([3, 4]). Moreover, the multizone combustion approach has been extended and modified for very high premixed combustion processes.

The use of a nonstationary 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 shown in [3]. Moreover, the nonstationary model also allows the “entrainment wave” effect ([3]) to be considered. This effect almost doubles the air entrainment in the spray after closure of the injector nozzle compared to the steady-state solution. The entrainment wave effect has a significant impact on the equivalence ratio distribution in the spray in all cases in which combustion starts at the end, or after the end, of injection, as in the burning of pilot injections or in high premixed combustion cases.

The other novelties of the present paper concern: the implementation of post-combustion mixing and cooling submodels for the burned gases produced from diffusive combustion; application of the approach to investigate the effects of rail pressure, the number of injection shots, and the DT between the pilot and main injections, on combustion and emissions, with emphasis on the soot formation process.

MODEL DESCRIPTION

1D SPRAY MODEL

For a complete description of the 1D spray model and for the 1D spray model assumptions, the reader should refer to [3, 4]. Basically, the spray for each injector nozzle hole is modeled as a cone, which is characterized by a spreading angle θ .

The fuel is considered non-vaporizing. However, as reported in [3, 4], “the equivalence ratio solution of the non-vaporizing model described below can also predict mixing limited liquid-fuel vaporization behavior”. In [4], it is also shown that, if the spreading angle θ is chosen adequately (see Eq. (11) in this paper and the related comments), the spray penetration and the cross-section mixture fraction calculated by the non vaporizing spray model are very close to the experimental ones obtained for a vaporizing spray.

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 (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:

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

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

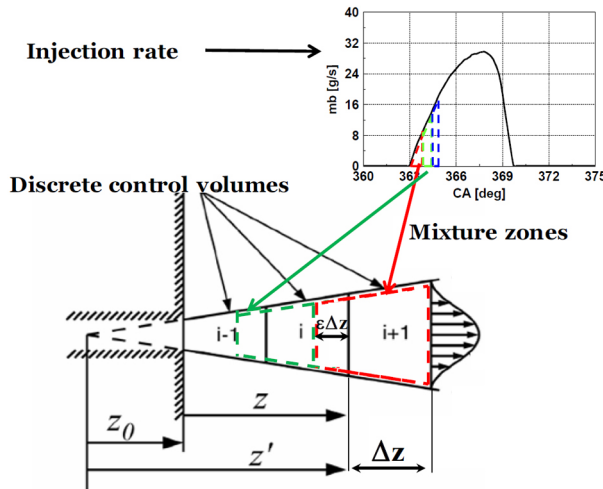


Figure 1. Scheme of the spray conic region in which the discrete control volumes and the mixture zones are reported, along with an injection rate example (top).

By assuming a proper distribution of the turbulent mean fuel volume fraction $\bar{X}_f$, and of the turbulent mean velocity $\bar{u}$ ([3, 4]), 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 $\dot{M}$:

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

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

$$\text{where } \beta = \frac{6(\alpha+1)(\alpha+22)}{(3\alpha+2)(2\alpha+1)}.$$

The β parameter is introduced to take into account 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.

Eq. (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 considered to be available from the experimental characterization of the injectors, in order to calculate the fuel velocity value 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, according to [11]:

$$\tan\left(\frac{\theta}{2}\right) = c \left[\left(\frac{\rho_u}{\rho_f} \right)^{0.19} - 0.0043 \sqrt{\frac{\rho_f}{\rho_u}} \right] \quad (11)$$

where c mainly depends on the nozzle orifice diameter ([12]).

A constant spreading angle, which was calculated by taking the in-chamber conditions at the SOL (start of

injection) instant into account, was considered for each injection pulse. In the case of a high dwell-time, two separate conic regions with different spreading angles θ are used for the pilot and main contributions, respectively. In the case of a reduced dwell-time, a single conic region with a constant spreading angle θ is used for the pilot and main injections in the 1D spray model. The spreading angle is not expected to vary significantly between the pilot and main for a reduced dwell-time.

It was found that using the total number of control volumes 'i' adopted in the 1D spray model in the multizone thermodynamic combustion model led 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 into equal portions. The unburned gas entrainment in each mixture zone is governed by the solution of the 1D spray model. It is clear that each mixture zone could occupy more than one control volume of the 1D spray model. In order to integrate the information derived from the 1D nonstationary spray model with the multizone combustion diagnostic approach, it is necessary to calculate the mixing process of each injected fuel parcel with the surrounding unburned gas as a function of time and the axial position.

The procedure is graphically and qualitatively illustrated in Figs. 1-2. The lower part of Fig. 1 reports a scheme 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 upper 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 lower 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 injection tip (the lower 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. This is shown

in Fig. 2, which reports ϕ in the conic spray region as a function of the axial distance for three different time instants after SOI. The colored portions below the ϕ distribution in

Fig. 2 also show the locations of the mixture zones along the spray axis at each time instant.

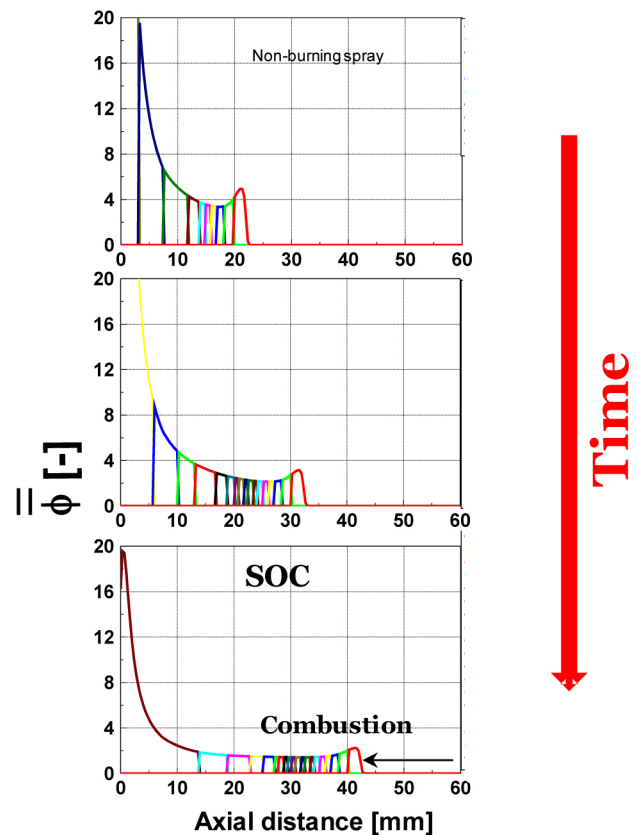


Figure 2. Distribution of ϕ along the axial spray distance for different time instants until SOC (bottom graph). The splitting of the spray into mixture zones is also indicated.

If the jet penetration is known at each time instant (corresponding to the last control volume in which the spray velocity 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 (Fig. 2). The fuel mass which is involved (and thus the mixture zones) is

derived using the multizone diagnostic approach (i.e., it is driven by the in-cylinder pressure time history).

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. As shown in [2, 8], 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:

$$d\lambda_j = (d\lambda_j)_{1D} \left[1 - \frac{m_{f,burned} (1 + \alpha_{st}^u)}{m^*} \right] \quad (12)$$

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.

Case 1. The whole mixture is lean/stoichiometric.

In this case, the fuel chemical energy can be released completely during the premixed burning. This is usually the case of pilot injection shots, the burning of which generally starts after the end of injection. This kind of combustion was analyzed and illustrated in [13] by means of laser-sheet imaging. In this case, the two-stage concept of a rich premixed combustion, with a soot formation region in the inner part of the spray, surrounded by a stoichiometric thin diffusion flame at the jet periphery, is no longer valid, since the experimental tests show that the entire jet cross-section burns in premixed stoichiometric/lean combustion conditions without soot formation. Soot would only be formed at the very end of the spray, in case in which the head vortex interacts with the cylinder wall. The stoichiometric/lean values of ϕ inside the jet are justified by the entrainment wave phenomena ([3]), which increase the ambient gas entrainment in the spray to a great extent after the end of injection and before the start of combustion. This conceptual scheme can also occur for the main pulse, when highly premixed combustion concepts are considered or when low-load operations are investigated in conventional diesel engines. For these cases, the HRR usually peaks long after the end of injection, or the combustion starts after the end of injection ([13]). The entrainment wave phenomena ([3]) determine a high entrainment rate of the unburned gas in the

spray at the beginning of combustion, and a stoichiometric/lean premixed combustion is expected to occur.

Case 2. The whole air-to-fuel mixture ratio is rich.

In this case, the fuel chemical energy can only be released completely through the two-stage premixed-diffusive conceptual scheme. This is the typical case of a main injection in which the HRR peak occurs well before the end of injection. All the fuel parcels undergo a rich premixed phase, whose combustion products complete oxidation in a thin diffusion flame at the jet periphery. This is consistent with the analysis reported in [14], in which the inner part of the burning spray is characterized by the presence of soot, as a consequence of rich premixed combustion; the premixed combustion products complete oxidation at the jet periphery through a diffusion flame. This situation has generally been verified to occur at medium-high load cases.

Case 3.

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, whereas the parcels that are injected later on have sufficient time to reach stoichiometric/lean conditions before oxidation. This usually occurs in the main injection pulses in which the HRR peaks near the end of the main injection. In this case (see [14]), it has been shown that the jet structure is characterized by two regions: an advanced region, in which soot formation has occurred as a consequence of the rich premixed combustion of the first injected parcels ([2]), and the remaining upstream jet, which is characterized by stoichiometric/lean combustion without the formation of soot.

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 CO₂ 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 [5], 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. The SOPC of the injection shot that follows the first one, which can be a second pilot or the main injection, is calculated as the instant at which the mixture zones of the previous injection pulse are consumed completely. The mixture zones of the following injection shot start oxidizing from this instant onwards.

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

For case 1, in which the main combustion starts after EOI, or the HRR peak occurs after EOI, combustion usually occurs in fully premixed conditions, with values of the equivalence ratio, derived from the 1D spray model, that are generally found to be stoichiometric/lean. Therefore, no SODC is detected.

In case 2 (two-stage premixed-diffusive burning), a 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 deg after the SOPC. A procedure for the estimation of SODC for this kind of case was proposed in [2], where it was observed that, if the oxidation rate derived from the pressure signal is only assigned to the premixed combustion, all the rich mixture zones are oxidized at a crank angle before the end of injection, and this causes the elaboration to stop. As a consequence, a fraction of the HRR must be derived from diffusive combustion, which should therefore start before that angle. A limiting crank angle, below which the mixture zones are not completely consumed before the end of injection, has been verified to exist, by an iterative procedure, for the onset of diffusive combustion. This angle was assumed as the SODC, and can be considered as the instant at which the rich premixed combustion products of the first injected fuel parcels reach stoichiometric conditions at the jet periphery. With this procedure, the SODC was found to occur at about 3 deg after SOPC in [2]. This can be considered as a quite reasonable value compared to the values found in [16] which are based on experimental laser sheet experiments. An assumption has to be made from the SODC to evaluate the contributions of the premixed and diffusive combustion to the total HRR. The assumption in [2] was that the mass oxidation rate of the premixed combustion, after the onset of the SODC, was kept constant and equal to that of the SODC.

For case 3 (in which the HRR peak is near the end of injection), it was found in [2] that, after the SOPC of the main, which starts in rich conditions, the not yet oxidized mixture zones become stoichiometric before they are consumed. In these cases, only the first injected mixture zones that burn in rich conditions are assumed to deliver mass to the rich premixed burned gas zone, which later oxidizes in the diffusive zones, whereas the not yet oxidized stoichiometric mixture zones are assumed to deliver mass directly to the diffusive burned gas zones. The instant at which the not yet oxidized mixture zones become stoichiometric is assumed as 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 trace, 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 ($dt = d\theta / \omega$) can be written as follows:

$$\delta Q + V dp = dI + |\dot{I}_{out}| dt - |\dot{I}_{in}| dt \quad (13)$$

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:

$$\delta Q_u + V_u dp = m_u di_u \quad (14)$$

$$\delta Q_{m,k_j} + V_{m,k_j} dp = m_{m,k_j} di_{m,k_j} + dm_{f,inj} (i_{m,k_j} - i_{f,I}) + dm_{u \rightarrow m,k_j} (i_{m,k_j} - i_u) \quad (1 \leq k_j \leq M_j) ; (1 \leq j \leq J) \quad (15)$$

$$\delta Q_{bp,j} + V_{bp,j} dp = m_{bp,j} di_{bp,j} + \sum_{k_j=1}^{M_j} dm_{m,k_j \rightarrow bp,j} (i_{bp,j} - i_{m,k_j}) \quad (1 \leq j \leq J) \quad (16)$$

$$\delta Q_{bd,h_j} + V_{bd,h_j} dp = m_{bd,h_j} di_{bd,h_j} + dm_{u \rightarrow bd,h_j} (i_{bd,h_j} - i_u) \quad (1 \leq h_j < N_j) ; (1 \leq j \leq J) \quad (17)$$

$$\begin{aligned} \delta Q_{bd,N_j} + V_{bd,N_j} dp = m_{bd,N_j} di_{bd,N_j} + \\ + dm_{bp,j \rightarrow bd,N_j} (i_{bd,N_j} - i_{bp,j}) + \\ + dm_{u \rightarrow bd,N_j} (i_{bd,N_j} - i_u) \quad (1 \leq j \leq J) \end{aligned} \quad (18)$$

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.

Figure 3 reports a conceptual combustion scheme considering case 2, in which the multizone approach zones and the mass-exchange between the zones are also reported.

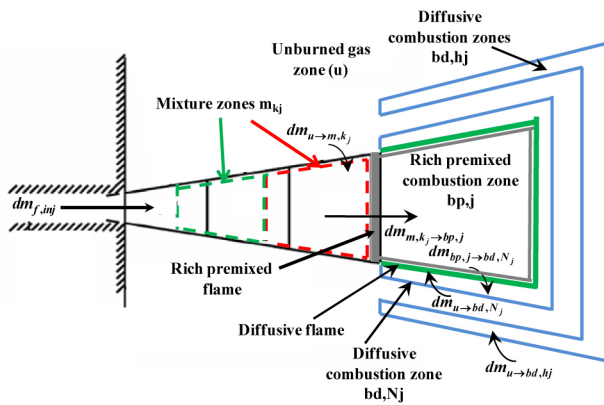


Figure 3. Conceptual combustion scheme for case 2 (two-stage premixed-diffusive burning). The mass-exchange between zones is also indicated.

In Eq. (15), $dm_{f,inj}$ indicates the mass of injected fuel in the dt interval, whereas the mass of unburned gas $dm_{u \rightarrow m,kj}$, which enters the mixture zone in the time interval dt , is obtained from the 1D spray model. If the time history of $\phi_{m,kj}$ is known, one obtains:

$$dm_{u \rightarrow m,kj} = \alpha_{st}^u \left[\frac{m_{m,kj}^f(t+dt)}{\phi_{m,kj}(t+dt)} - \frac{m_{m,kj}^f(t)}{\phi_{m,kj}(t)} \right] \quad (19)$$

where $m_{m,kj}^f$ is the mass of fuel in the mixture zone m,kj at the considered time instant, which is obtained from the injection rate and from the number of generated mixture zones into which the total injected fuel is split. The term $dm_{m,kj \rightarrow bp,j}$ in Eq. (16) indicates the m,kj mixture zone mass which enters the premixed bp,j zone as a consequence of the premixed combustion. If the heat release is only due to premixed combustion, the term $dm_{m,kj \rightarrow bp,j}$ is derived from the solution of the mass and energy equation system, and is governed by the experimental in-cylinder pressure signal. The

term $dm_{u \rightarrow bd,hj}$ in Eq. (17) is the unburned gas mass which enters the diffusive burned gas zones bd,hj as a consequence of the dilution effect. If a dilution model, which provides the value of $\lambda_{bd,hj}$ as a function of time, is considered, $dm_{u \rightarrow bd,hj}$ can be calculated as follows:

$$\begin{aligned} dm_{u \rightarrow bd,hj} &= \alpha_{st}^u \left[\lambda_{bd,hj}(t+dt) - \lambda_{bd,hj}(t) \right] m_{bd,hj}^f = \\ &= \alpha_{st}^u \left[\lambda_{bd,hj}(t+dt) - \lambda_{bd,hj}(t) \right] \frac{Q_{ch,bd,hj}}{LHV} = \end{aligned} \quad (20)$$

where $m_{bd,hj}^f$ is the mass of fuel associated with the zone bd,hj which has burned in diffusive combustion, and released the total chemical energy $Q_{ch,bd,hj}$; LHV is the fuel lower heating value. Finally, in Eq. (18), $dm_{bp,j \rightarrow bd,Nj}$ is the mass of the premixed combustion products that enters the diffusive burned gas zone Nj after the onset of diffusive combustion. This mass is calculated at each instant by solving the set of mass and energy conservation equations, and it is governed by the experimental in-cylinder pressure signal. Since diffusive combustion occurs in stoichiometric conditions, the $dm_{bp,j \rightarrow bd,Nj}$ mass requires a $dm_{u \rightarrow bd,Nj}$ mass of unburned gas in order to reach stoichiometric conditions. This mass can be calculated as reported in [5], on the basis of the following relation

$$dm_{u \rightarrow bd,Nj} = \frac{dm_{bp,j \rightarrow bd,Nj}}{1 + \overline{\alpha_{bp,j}^u}} \left(\alpha_{st}^u - \overline{\alpha_{bp,j}^u} \right) \quad (21)$$

where $\overline{\alpha_{bp,j}^u}$ indicates the averaged unburned gas/fuel ratio of the premixed burned gas zone, i.e. the ratio of unburned gas and fuel which, after combustion, has generated the premixed burned gas products of the bp,j zone at the considered time

instant (see [5]). Equation (21) indicates that the lower $\overline{\alpha_{bp,j}^u}$ (due to a richer combustion), the higher the mass of unburned gas required to reach stoichiometric conditions for diffusive combustion.

The enthalpy convection terms on the right hand side of Eqs. (15, 16, 17, 18) 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 products of rich premixed combustion complete their oxidation. The diffusive burned gas zones Nj 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