

A Physical 0D Diesel Combustion Model Using Tabulated Chemistry with Presumed Probability Density Function Approach: For engine pre-Mapping

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ABSTRACT – This paper presents a new 0D phenomenological approach to predict the combustion process in Diesel engines operated under various running conditions. The aim of this work is to develop a physical approach in order to improve the prediction of in-cylinder pressure and heat release for developing a tool for engine pre-mapping. The main contribution of this study is the modeling of the premixed part of the Diesel combustion.

In phenomenological Diesel combustion models, the premixed combustion phase is sometimes modeled as the propagation of a turbulent flame front. However, experimental studies have shown that this phase of Diesel combustion is actually a rapid combustion of part of the fuel injected and mixed with the surrounding gas. This mixture ignites quasi instantaneously when favorable thermodynamic conditions are locally reached. A chemical process then controls this combustion.

In the present model, the rate of heat release by combustion for the premixed phase is related to the mean reaction rate of fuel. The latter is evaluated by an approach based on tabulated local reaction rate of fuel and on the determination of the Probability Density Function (PDF) of the mixture fraction (Z), in order to take into consideration the local variations of the fuel-air ratio. The shape of the PDF is presumed with a standardized β -function. Mixture fraction fluctuations are described by using a differential equation for the variance of Z . The standard mixture fraction concept established in the case of diffusion flames is here adapted to premixed combustion to describe the inhomogeneity of the fuel-air ratio in the control volume. The detailed chemistry is described using a tabulated database for reaction rates and cool flame ignition delay as a function of the progress variable c .

Premixed zone volume and total entrained ambient gas mass flow rate are calculated using a detailed spray model. The mixing-controlled combustion model is based on the calculation of a characteristic mixing frequency which is a function of the turbulence density, and on the evolution of the available fuel vapor mass in the control volume.

The developed combustion model is one sub-model of a thermodynamic model based on the mathematical formulation of the conventional two-zone approach. This zero-dimensional model incorporates several sub-models describing turbulence, vaporization, and fuel introduction rate. The purpose of this approach is to directly relate physical model parameters to operating conditions and engine parameters.

Numerical results from simulations are compared with experimental measurements carried out on a 2 liter Renault Diesel engine. For all investigated operating conditions, simulated cylinder pressure and heat release rate traces show a good agreement with experimental data.

INTRODUCTION

During recent years, considerable improvements of High Speed Direct Injection Diesel Engine technology have been made, with a strong increase of fuel economy and a remarkable reduction of emissions and combustion noise. These improvements have been achieved with

the introduction of complex system-layouts involving a large number of devices such as EGR system or Common Rail Direct Injection System. New strategies in Diesel combustion tend to use HCCI (Homogeneous Charge Compression Ignition) combustion modes more and more. Furthermore, it has been highlighted that combustions resulting from pilot injections in multi-injection strategies correspond to premixed combustions [1].

These latest developments in engine technology involve strong development of engine models to describe the effects of fuel injection systems on the combustion process. Numerical simulation plays an increasingly important role in the development process of internal combustion engines. The 0D phenomenological models are at the turning point between CFD 2D/3D model and look-up table models. Improvement of physical representative capability while keeping reasonable CPU performances in order to be embedded in a full engine simulator is a challenging and relevant topic in 0D model development. The well known pioneers of this kind of models for Diesel combustion are Barba et al. [2] and Chmela et al. [3, 4], but their contributions have mainly focused on specific applications. Therefore, their models are not able to directly represent the complexity of the current challenges such as quasi HCCI combustion, multi injection strategies or combustion with high EGR rate. Phenomenological 0D engine models are of particular relevance to perform a large number of numerical tests at costs that are much lower than those associated with experiments. The aim of this work is to develop a physical approach for combustion modeling in Diesel engines. The major challenge for the combustion model consists in precisely describing the overall engine operating conditions. In DI Diesel combustion, premixed combustion is characterized by an air/fuel ratio distribution inside the spray volume, more or less homogeneous according to time after injection and mixture velocity [1]. The first auto-ignition site appears inside the spray, where chemical and thermodynamic conditions are the most favorable. In this paper, the air/fuel ratio stratification inside the spray region is described by a presumed PDF (Probability Density Function) approach [5]. The diffusion combustion model is based on the Barba et al. [2] approach, in which the heat release rate is described with a characteristic mixing frequency. The developed model is able to accurately predict the combustion process for a wide range of operating parameters, while requiring low CPU resources.

THE PHENOMENOLOGICAL COMBUSTION MODEL

The description of the thermodynamic conditions in the combustion chamber is based on a mathematical formulation of the conventional two-zone approach. This zero-dimensional thermodynamic model assumes that at any time during the combustion process, the cylinder volume is divided into two zones, corresponding to burned and unburned gas regions. In each zone the thermodynamic state is defined by the means of thermodynamic properties and the specific heat of each gas component changes according to the approximated formula from the JANAF thermodynamic properties table. Unburned gas composition corresponds to dry surrounding air (N_2 , O_2 , Ar, CO_2) with fuel vapor (n-heptane C_7H_{16}) Burned gas mixture composition results from a stoichiometric combustion equation (N_2 , H_2O , Ar, CO_2). Both zones are assumed to have the same uniform in-cylinder pressure. The unburned mixture and burned mixture zones are each treated as separate open systems, with mass transfer and variable composition, and the governing equations are the mass and energy conservation equations and ideal gas equation of state. Mass flow rate in each zone is deduced from a balance equation corresponding to mass transfer through intake and exhaust valves, mass transfer between the two zones due to combustion and fuel injection rate in the unburned gas zone.

The quasi-dimensional thermodynamic model incorporates several sub-models to take into account several physical phenomena (turbulence, vaporization, spray and entrained gas mass flow rate), represented in Figure 1.

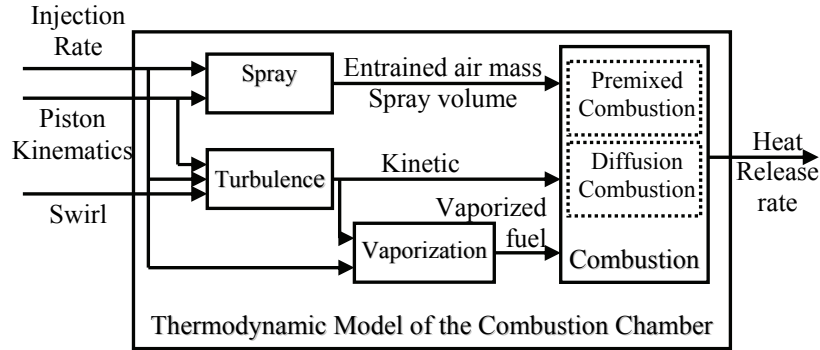


Figure 1: Basic principle of combustion chamber model

Spray and entrained surrounding gas model

This model provides the geometrical characteristics of the spray with a perfect cone shape assumption. The spray model is based on the approach developed by Siebers et al. [6, 7], which is a theoretical approach for the evaluation of the penetration of a non-vaporizing ideal liquid spray. The entrained surrounding gas model is based on mass and momentum conservation laws. Spray velocity is assumed decreasing with the surrounding air entrainment in the spray volume. The main assumption is air + EGR mixture density is assumed to be very close to the total density in the combustion chamber: $\rho_a \approx \rho$. Thus the entrained gas mass flow rate into the spray zone can be written as:

$$\dot{m}_{a,s} = \rho \dot{V}_s - \frac{(V_{cyl} - V_s)}{V_{cyl}} \dot{m}_{cyl} - \rho \frac{V_s}{V_{cyl}} \dot{V}_{cyl} \quad (1)$$

With V_{cyl} and V_s being the chamber volume and the spray volume respectively, \dot{V}_{cyl} results from the piston kinematics and \dot{V}_s results from the spray sub model.

Two states turbulence model: K-k modified model

Chmela and Orthaber [3, 4] propose that the influence of the spray kinetic energy, compared to the other production terms, is dominating and thus assume that the other terms are negligible. Indeed, the production of turbulence is mainly due to a strong shear at large scale between spray and surrounding gas in the combustion chamber. But newer engines implement technologies such as swirl flaps which produce large swirl numbers. Thus, the model must take into account combustion subjected to large swirl numbers that influence average movement in the combustion chamber. Swirl which is used for pollution control (soot and particulate emission) affects the mixing rate. Two control volumes are then considered in energy balance equations, as described on Figure 2. Firstly, in the combustion chamber volume, swirl creates a flow and the associated kinetic energy. After the start of injection swirl dissipates energy in the spray volume, resulting in spray deformation, and kinetic energy associated with the average movement is increased. In the second volume, there are two main steps. At first, the kinetic energy associated to the mean movement is transferred to the fluctuating movement and creates turbulent kinetic energy at large scale. Then, this turbulent kinetic energy is transferred to small scales and is dissipated by viscous friction.

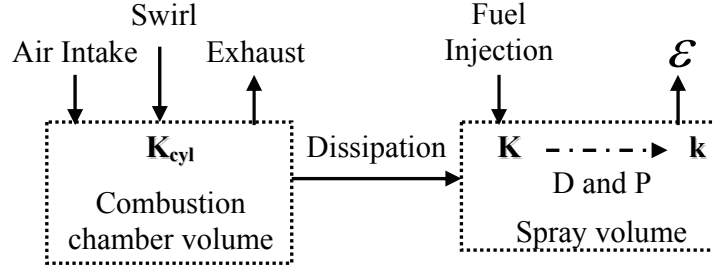


Figure 2: Diagram of the energy balance in the combustion chamber

For total flow in the combustion chamber, the kinetic energy associated with the average movement is [8, 9]:

$$\frac{dK_{cyl}}{dt} = C_{int} \left(\frac{1}{2} \dot{m}_{int} v_{int}^2 \right) + C_{exh} \left(\frac{1}{2} \dot{m}_{exh} v_{exh}^2 \right) + \left. \frac{dK_{swirl}}{dt} \right|_{prod} + K_{cyl} \frac{\dot{m}_{exh}}{m} - \left. \frac{dK_{cyl}}{dt} \right|_{diss} \quad (2)$$

In the above equation, m is the total mass in the cylinder and K_{cyl} production terms are mainly related to the kinetic energy of intake, exhaust flows and swirl.

Now the control volume corresponds to the spray volume. The assumption for the energy balance equation in the spray volume is that swirl does not induce mass transfer between the surrounding air and the spray volume, but only dissipates energy. By writing the energy conservation equations, the rate of kinetic energy of average and turbulent movement in the spray are [8, 9]:

$$\frac{dK}{dt} = \left. \frac{dE_{kin}}{dt} \right|_{inj} + \left. \frac{dK_{cyl}}{dt} \right|_{diss} + K \frac{\dot{m}_{exh}}{m} + K \frac{\dot{\rho}}{\rho} - P \quad (3)$$

$$\frac{dk}{dt} = P - D + k \frac{\dot{m}_{exh}}{m} + k \frac{\dot{\rho}}{\rho} \quad (4)$$

With the production and dissipation terms, $P = c_p K/t_p$, $D = c_D k/t_D$, and characteristic times: $t_p = L_I/U_f$, $t_D = L_I/u'$. The integral length scale L_I is assumed proportional to a characteristic dimension of the combustion chamber, $L_I = c_L \sqrt[3]{V_{cyl}}$.

Vaporization model

Fuel vaporization in a 0D approach is modeled by the interaction between fuel droplets and their environment. The spray expansion, aerodynamics, temperature and gas composition in the combustion chamber have a large influence on fuel vaporization. Three approaches are mainly used in the literature: the overall vaporization model, the model based on the “d²” law and the isolated droplet model. The first approach was selected because less CPU time is required. It consists in a global first order model vaporizing the liquid fuel according to a characteristic time τ_{vap} [3].

Premixed Combustion Model

The accurate description of the premixed combustion is important especially in part load conditions or in multi injection strategies. Indeed, for single injection tests with low torque and strongly diluted conditions, the majority of the fuel vapor burns in premixed mode. The premixed combustion influences the diffusion combustion by consuming a great part of the injected and vaporized fuel. The same phenomenon occurs for pilot combustion in the case of multi injection strategies. The fuel mass burned in the pilot combustion must be known for an

accurate description of the main combustion. One of the main issues in conventional Diesel combustion modeling is that auto-ignition takes place in stratified-mixture conditions. In this work, the premixed combustion mode is modeled assuming that the reaction mechanism, which controls premixed combustion, is similar to the one that takes place during ignition delay. Consequently, for modeling this part of combustion, a detailed chemistry-based auto-ignition model including low temperature phenomena is used to compute a local reaction rate of fuel. The importance of chemical kinetics in new injection strategies in conventional Diesel engines does not allow the use of classical Diesel auto-ignition models based on oversimplified representations of the chemistry such as those found in Barba et al. [2]. The tabulation method [10, 11, 12] adopted in this work has been originally developed for the 3D internal combustion engine calculations ECFM3Z model [13] and here adapted for the 0D approach. Moreover in DI Diesel engines, an equivalence ratio gradient exists across the spray volume. Due to the non-linear dependency for the reaction rate of fuel on equivalence ratio, the equivalence ratio distribution, which develops in the surrounding gas, must be considered to correctly estimate the rate of heat release by combustion. Thus, in the present model, the mean reaction rate of fuel is evaluated by an approach based on the determination of the Probability Density Function of the mixture fraction $Z \in [0,1]$. The mean reaction rate associated to fuel is given by the convolution product between the local reaction rate of fuel $\dot{\omega}_f$, determined by tabulation, and the probability density function of the mixture in the control volume $P_{\tilde{Z}, \tilde{Z}^2}(Z)$:

$$\bar{\dot{\omega}}_f = \int_0^1 P_{\tilde{Z}, \tilde{Z}^2}(Z) \dot{\omega}_f(Z) dZ \quad (5)$$

Equation (5) is obtained according to several assumptions [14, 15]: temperature, pressure and EGR mass fraction are considered homogeneous in the spray volume, and the progress variable c is assumed homogeneous during combustion, i.e. $c(Z) = \tilde{c}$, $\forall Z$. Thanks to these assumptions the general form of the joint PDF [14, 15] is reduced to a simple single variable PDF. In [14], the impact of this assumption on the combustion process is discussed and it is shown that the auto ignition process is not affected. The rate of fuel mass consumed by the premixed combustion is:

$$\dot{m}_{f,comb,pre} = \bar{\dot{\omega}}_f m_{f,pre} \quad (6)$$

$m_{f,pre}$ is the mass of the vaporized fuel available for premixed combustion. Due to the air/fuel ratio distribution in the spray, the heat release of the premixed fraction in DI Diesel engine is not instantaneous. There exist multiple ignition spots due to local thermodynamic properties and concentration evolution. With conventional approaches in 0D modeling, each zone is defined homogeneous [16]. With new combustion modes, this assumption is not sufficient to accurately calculate an auto-ignition delay or a reaction rate. This work makes use of a statistical approach which consists in presuming the shape of the stratified zone with a probability density function. Non homogeneous mixing between fuel vapor and surrounding gas is presumed with a standardized β -function PDF shape. The mixture fraction definition has been used to describe the equivalence ratio distribution in the spray zone. The mean value of the mixture fraction, which is constant during combustion, is:

$$\tilde{Z} = \frac{\gamma Y_{f,s} - Y_{O_2,s} + Y_{O_2,a,nm}}{\gamma + Y_{O_2,a,nm}} \quad (7)$$

$Y_{f,s}$ is the mass fraction of fuel in the spray volume, $Y_{O_2,s}$ is the mass fraction of oxygen in the spray volume and $Y_{O_2,a,nm}$ is the mass fraction of oxygen in the not-mixed zone. \tilde{Z}^2 quantifies the mixture fraction fluctuations, in the unburned gas mixture, related to mixing. Deriving the probabilistic definition of the mixture fraction variance, Mauviot [1, 14] relates statistical

variables to physical phenomena through a transport equation. The obtained equation (8) distinguishes three contributions influencing the mixture. The first term corresponds to the vaporized fuel flow contribution, the second term corresponds to the entrained air mass flow contribution, and the third term corresponds to the dissipation. This term is the micro mixing process contribution and indicates that the mixture is directly related to turbulence inside the chamber. The first two terms increases the variance whereas the last term decreases it.

$$\frac{d\widetilde{Z}^2}{dt} = \underbrace{\frac{1}{m_s} \left[(1 - \widetilde{Z})^2 - \widetilde{Z}^2 \right] \dot{m}_{vap}}_{\text{Term relate to evaporated fuel flow}} + \underbrace{\frac{1}{m_s} (\widetilde{Z}^2 - \widetilde{Z}^2) \dot{m}_{a,s}}_{\text{Term related to entrained air flow}} - \underbrace{2C_\Phi \frac{\widetilde{Z}^2}{k/\varepsilon}}_{\text{Dissipation Term}} \quad (8)$$

In this equation, m_s is the sum of the gaseous fuel mass plus the mass of entrained air in the spray, \dot{m}_{vap} is the vaporized fuel flow given by the vaporization sub-model, $\dot{m}_{a,s}$ is the entrained surrounding air flow into the spray volume given by equation (1). C_Φ is a constant parameter linked to turbulence that has to be adjusted.

Diffusion Combustion Model

The second part of the combustion model is the diffusion or mixing-controlled combustion model. This combustion mode is based on the approach developed by Barba et al. [2]. For engine operating conditions corresponding to full load and with several pilot injections, the main combustion is principally a mixing-controlled flame. This phenomenon, which is controlled by the mixing between surrounding air and fuel vapor, is slower than the premixed combustion. Common zero-dimensional diffusion models are based on the available fuel vapor mass enclosed in the control volume and on a characteristic mixing frequency which is a function of the turbulence density. Thus the fuel mass consumed by the diffusion combustion is:

$$\dot{m}_{f,comb,diff} = F_{mix} \frac{\sqrt{C_{V_{MP}} V_{MP}^2 + C_k k}}{\sqrt[3]{\frac{\Phi V_{cyl}}{n_N}}} m_{f,diff} \quad (9)$$

With $m_{f,diff}$ the mass of the vaporized fuel available for diffusion combustion, F_{mix} is an empirical function defined by Barba et al. [2] to take into account a delay between start of premixed combustion and start of diffusion combustion. $C_{V_{MP}}$ and C_k are two parameters which are optimized using a limited number of operating points by matching the simulated combustion results with experimental heat release profiles. The determined values are then kept constant for all the engine operating conditions.

Extended Model for Multi Injection

In the developed approach for multi-injection strategies, each injection leads to a spray model, a vaporization model and a combustion model. Only the turbulence model is an overall model and each injection increases the turbulence inside the combustion chamber. For each injection, models are computed with the surrounding conditions at injection timing. Gas entrained into the spray zone comes not only from the unburned gas zone but also from the burned gas zone:

$$m_{a,s} = Y_b m_b + (1 - Y_b) m_u \quad (10)$$

Where Y_b is the burned mass fraction, m_b and m_u are, respectively, the burned and unburned air mass computed with the thermodynamic model. In this extended model, the main

assumption is the instantaneous mixing between unburned and burned gases. This model is therefore more suited for an injection pattern where injections are not too close to each other. A short time perspective to improve this model is to develop another sub-model to take into account interactions between the sprays. Nevertheless, most of the time, this assumption appears sufficient to reproduce the effect due to the pilot combustion on main combustion. The limits of this assumption are reached for cases with large swirl number or for split injections. In these cases it is possible to inject directly into a zone composed only by burned gas, which is not taken into account by the vaporization model and by the presumed PDF model for premixed combustion. The interaction between successive injections is done with the dissipation term in equation (8) and with the quantity of burned gas entrained into the spray volume. Finally, tabulation input parameters for the local reaction rate evaluation (pressure, equivalence ratio and fraction of dilution gases) are computed for each injection by taking into account their variation due to the combustion of the previous injection.

RESULTS AND DISCUSSION

In this section, measured engine data are compared with computed results using the developed combustion model. The various experimental measurements were carried out on a two-liter Renault Diesel engine with a 16.2:1 compression ratio, equipped with a common rail injection system. Injection rates are modeled with Hermits polynomials optimized for each injection. The overall combustion chamber model is calibrated with a limited number of operating points, using the experimental data provided by the engine bench. The determined model parameters are then kept constant for the whole range of engine operating parameters. The global methodology consists in separating the different sub-models calibrations. Therefore in order to limit the interactions, each model is calibrated on specific operating points. To test the model predictivity a minimum set of engine tests is chosen, less than 10% of all available tests. In the following figures, the experimental apparent energy release rate is calculated from in-cylinder pressure traces and with the heat capacity ratio equal to 1.4. This experimental apparent energy rate is compared with the apparent energy rate calculated from the simulated pressure traces.

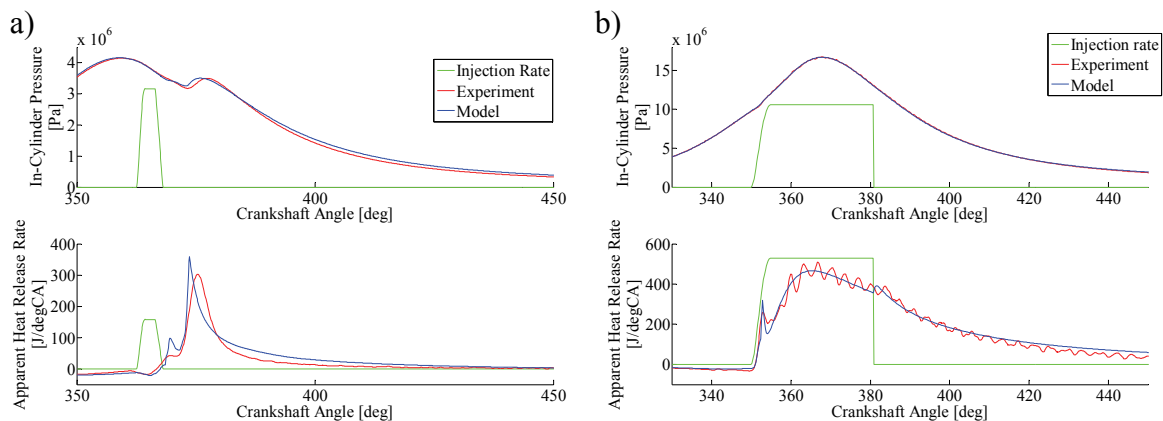


Figure 3: In-cylinder pressure and heat release rate as a function of crank angle degree for a single-injection test. a) At low-load and highly diluted, operating conditions: 1000rpm, IMEP=1bar, EGR rate 30.6%, b) At full-load, operating conditions: 4000rpm, IMEP=17.4bar, EGR rate 0.5%

Figure 3 shows that computed pressures and apparent heat release rate are in good agreement with experimental results for single injection tests. To validate the premixed combustion

model, an operating point providing long mixture duration before auto-ignition is used (Figure 3.a). In this case, after SOI and before AI, computed apparent energy rate shows a decrease due to fuel vaporization. This decrease is also observed on the experimental apparent energy rate. Simulated and experimental AI period are in good agreement and the first peak just after the AI, representative of the cool flame, is well reproduced by the model.

To validate the diffusion combustion model, a full-load test has been selected (Figure 3.b). Indeed under these operating conditions, the majority of the vaporized fuel burns in diffusion combustion mode. The mixing velocity is based on the evolution of the turbulent kinetic energy rate (equation (4)). After EOI, the production term of the kinetic energy, due to the injection rate, becomes null. Kinetic energy is then only dissipated resulting in the rate of heat release decrease.

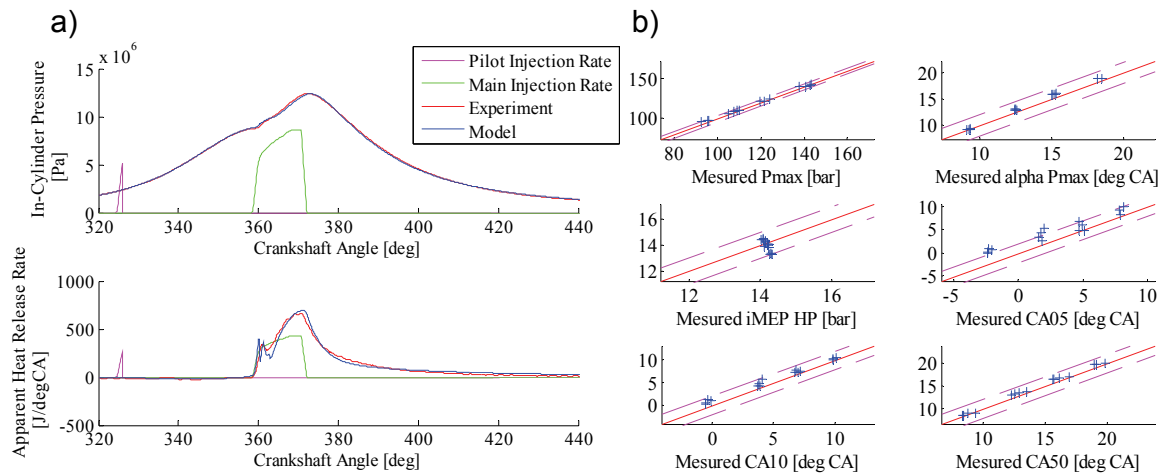


Figure 4: a) In-cylinder pressure and heat release rate as a function of crank angle degree for a multi-injection test at medium-load, operating conditions: 2250rpm, IMEP=12bar, EGR rate 30.6%. b) Predicted vs. measured combustion parameters for multi-injection tests at medium-load with EGR and SOI variation for the reference test represented in a). Dashed lines represent the maximum allowed values and tolerance ranges are, for $P_{max} \pm 4$ bars, for $\alpha P_{max} \pm 2$ CA, for $iMEP \pm 1$ bar, and for $CA_x \pm 2$ CA.

Figure 4.a shows that computed pressures and apparent heat release rates are in good agreement with experimental results for an experiment with two injections. This represented test includes one pilot injection early in the cycle and one main injection near the TDC. Figure 4.b shows results for pressure peak value, pressure peak position, IMEP values and crank angle values at which 5%, 10% and 50% of fuel is burned. These results are obtained for 12 multi-injection tests with EGR rate variations (0 to 20%) and with SOI variations for the main injection (-6 to +4°CA after the TDC). For each SOI, 4 values of EGR rate are used. These results have been obtained with the same set of parameters than the test represented in Figure 4.a.

To evaluate the overall combustion model, operating points covering the whole engine operating range have to be used (Figure 5). Indeed, the model is evaluated on several steady state operating points covering a large range of engine speeds, loads, EGR rate, and injection strategies representative of the whole engine application field.

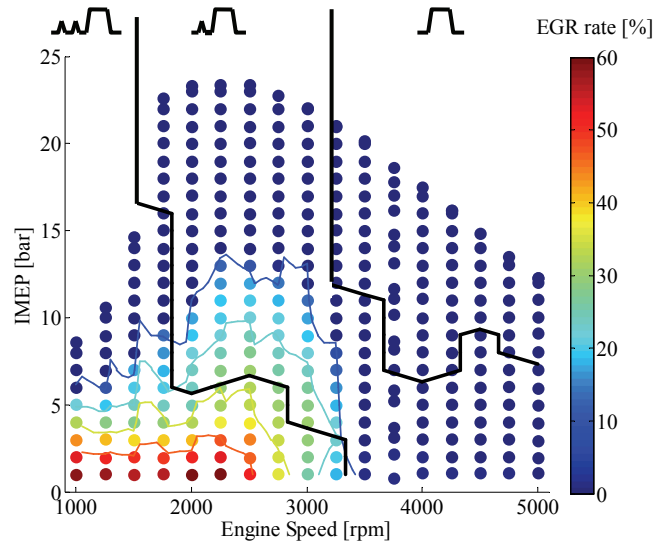


Figure 5: Set of experimental engine tests representative of the overall engine operating range (317 tests). In this figure, engine tests are identified with engine speed and IMEP and also with EGR rate and injection strategy.

The following figures present results for all tests, summarized in Figure 5, comparing the most important parameters in combustion prediction: peak pressure value, peak pressure position, IMEP values and the crank angle values at which 5%, 10% and 50% of fuel is burned.

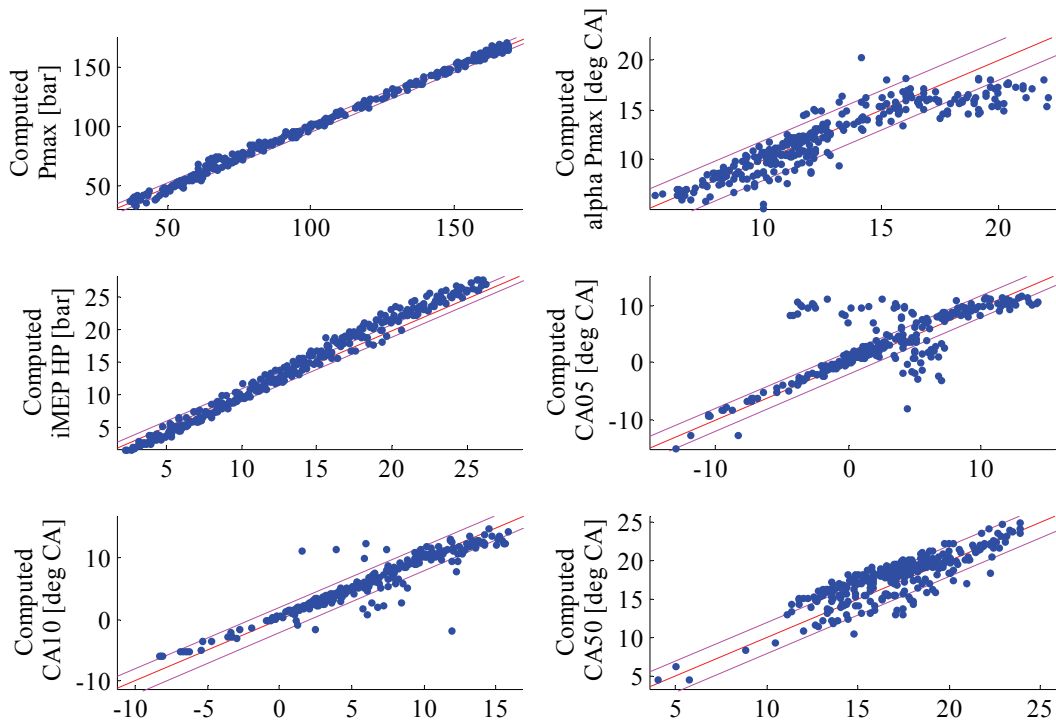


Figure 6: Predicted vs. measured combustion parameters for all tests resumed in Figure 5, magenta lines represent the maximum allowed values and red lines represent the perfect compatibility between predicted and measured parameters values. Tolerance ranges are, for $P_{max} \pm 4$ bars, for $\alpha P_{max} \pm 2$ CA, for $iMEP \pm 1$ bar, and for $CA_x \pm 2$ CA.

For all operating tests a good agreement is obtained. It is important to notice that the same set of parameters has been used in the combustion model for all of these tests. The difference

between the computed and measured values of iMEP is due to a bad modeling of the wall losses during expansion at the end of engine cycle. CA05 figure shows that some points are out of the tolerance range. For some of these tests, the crank angle value when five percent of fuel is burned is overestimated. This bad agreement corresponds to operating points where two pilot injections are used. As interaction between each injection is not taken into account by the model, auto ignition delay decrease of the main injection is not described for multi-injection tests. A better description of multi-injection is necessary to accurately model this kind of operating point. For some of the tests out of tolerance, the crank angle value when five percent of fuel is burned is underestimated. These tests correspond to late main injection timing, resulting in a possible interaction between spray and wall which is not taken into account by the model. Due to the bad evaluation of the vaporization rate, the available mass for combustion is then overestimated.

CONCLUSION

This paper presents an original approach for Diesel engine combustion modeling. The main contribution of this work is the new description of the premixed combustion phase. The premixed combustion model makes use of a statistical description of the air/fuel ratio distribution inside the spray region. EGR in the cylinder has an impact on chemical kinetics and cold flame phenomenon which can occur at the beginning of the fuel oxidation process. To answer these issues, the model uses complex-chemistry tabulation method in order to consider chemical kinetics.

Operating points with large mixing times have been used for model validation and a good agreement between experimental and computed values has been shown. For a wide range of engine operating points, simulated cylinder pressure and heat release rate traces show a good agreement with experimental measurements.

FUTURE WORK

The overall objective being the ability of the model to reproduce combustion modes ranging from conventional Diesel mode to full HCCI mode, future work should improve the model to take into account large EGR rates as well as in-cylinder temperature distribution. To improve the existing model, interaction between sprays must be taken into account in multi-injection cases. Furthermore, a more detailed spray model can improve general results especially in cases with multi-injection. Indeed, wall impingement and interaction between several sprays have an impact on combustion. A model for the mixing velocity between burned and unburned gases in the zone where injections take place, as a function of swirl number and kinetic energy rate, can be used.

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