

Validation and Application of a New 0D Flame/Wall Interaction Sub Model for SI Engines

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ABSTRACT

To improve the prediction of the combustion processes in spark ignition engines, a 0D flame/wall interaction submodel has been developed. A two-zones combustion model is implemented and the designed submodel for the flame/wall interaction is included. The flame/wall interaction phenomenon is conceived as a dimensionless function multiplying the burning rate equation. The submodel considers the cylinder shape and the flame surface that spreads inside the combustion chamber. The designed function represents the influence of the cylinder walls while the flame surface propagates across the cylinder. To determine the validity of the combustion model and the flame/wall interaction submodel, the system was tested using the available measurements on a 2 liter SI engine. The model was validated by comparing simulated cylinder pressure and energy release rate with measurements. A good agreement between the implemented model and the measurements was obtained.

INTRODUCTION

Modern automobile engines must fulfill challenging conditions in terms of efficiency and pollutant emissions while keeping performance. The answer to these constraints has been the development of new modes of combustion and the inclusion of mechanical devices such as turbochargers, variable valve timing (VVT) and exhaust gas recirculation (EGR). These new developments improve dramatically the engines performance, but their inclusion also results in a less predictable combustion, which might alter the proper functionality of the exhaust treatment systems. Studies in this area have coincided with the fact that in order to maintain the performance of these systems,

a more accurate prediction of the phenomenological combustion modeling is essential.

In the case of SI engines, several combustion models have been proposed, in most of them, the heat release is modeled by the classical turbulent premixed flame propagation. [1] provides a summary of different common combustion models. The main differences between the different propositions are associated with the modeling of the wrinkling phenomenon of the flame surface. Two different models were studied in this work: coherent flame model (CFM) and Fractal Combustion Model.

In [2], a 3D CFM model is developed. It describes the rate of fuel consumption per unit volume by the product of the flame surface density and the local speed at which it consumes the mixture. This model was reduced to 0D in [3]. In [4], [5] and [6], different fractal combustion models are proposed and the most relevant elements to characterize the fractal representation of the burning rate are developed. In this work, the fractal combustion model from [5] and its complement from [7] are implemented.

The previous 0D models mostly focus on the laminar characteristics and on the wrinkling phenomena of a free developing flame, but they lack a suitable approximation of the wrinkling phenomenon when the flame reaches the cylinder walls. The cylinder wall is a barrier that limits the fuel mobility. Besides, the wall temperature is colder when compared to the gases temperature, which decreases the gases expansion. These phenomena reduce the burning rate. This behavior might depend on the engine intake geometry, the combustion chamber geometry and the operating conditions [8]. Such a flame-wall interaction is an essential issue in accurately modeling the combustion process.

In this paper, a new model that takes into account the impact of the cylinder walls in the burning rate is proposed. This approach is based on the flame surface distribution with respect to the combustion chamber and the assumed linear decay during the flame-wall interaction. A well defined geometric model of the combustion chamber is designed in order to have more realistic results. The model is included in a 0D two-zones combustion model and can be included in several combustion schemes since it is conceived as a dimensionless function multiplying the burning rate equation. The model is tested taking as reference the available measurements on a 2 liters engine. It is validated with the data fit of the cylinder pressure and the energy release during the combustion.

In this paper the two zones thermodynamical model and the combustion model are described. A previous model to represent the combustion close to the walls is presented, this approximation was used before moving to the current approximation and will help to understand the improvements obtained with the main result of this work. Subsequently, the submodel to take into account the impact of the cylinder walls in the burning rate is illustrated, this model constitutes the main result of this work. Finally, comparison with experimental results are presented.

TWO ZONES THERMODYNAMICAL MODEL

There are some assumptions in the spark-ignition engine combustion process that permits a representation of this process with a two zones approximation [9]. Those assumptions are:

- the fuel, air and residual gases charge is uniformly premixed;
- the volume occupied by the reaction is small in comparison with the clearance volume, which means that the flame is a thin reaction sheet that becomes wrinkled as it develops.

Under these assumptions it can be assumed that the cylinder volume is divided into two zones: the burned gases and the unburned gases zones separated by the reaction layer. Each zone is defined by its mean thermodynamics properties and the specific heat of each gas component changes according to the JANAF thermodynamic properties table [10].

Both zones are assumed to have the same uniform in-cylinder pressure. The thermodynamical model describes the energy balance inside the combustion chamber. Each zone is considered as a separate open system. The mass flow rate into each zone is deduced from a balance equation corresponding to the mass transfer through intake and exhaust valves. The mass transfer between the two zones is modeled by the two zones combustion model detailed next.

The energy equation for each zone is inferred from [11] as:

$$dU_i = \delta Q_{th,i} - p dV_i + \left(\sum_j h_j dm_j \right)_i \quad (1)$$

where the subscript i denotes the zone: $i = b$ for burned gases or $i = u$ for unburned gases, U_i is the internal energy of the cylinder gas mixture, $\delta Q_{th,i}$ expresses the heat transfer of the cylinder contents to the surroundings, $p dV_i$ corresponds to the work delivered by the piston, $\sum_j h_j dm_j$ is the total energy flowing into or out of the zone i and h_i is the specific enthalpy of each zone.

The left hand side of (1) can be written as:

$$dU_i = u_i dm_i + m_i \sum_k u_{i,k} dY_{i,k} + m_i c_{v,i} dT_i \quad (2)$$

where $u_{i,k}$ is the internal energy of species k in the zone i and u_i corresponds to the internal energy of the whole mixture, $Y_{i,k}$ corresponds to the mass fraction of species k in the zone i . m_i is the total mass in zone i and T_i corresponds to the temperature of the mixture in the zone i .

Solving (1) and (2) for dT , two ordinary differential equations are implemented as governing equations for the system temperatures dynamics:

$$dT_u = \frac{1}{m_u c_{p,u}} \left(V_u dp - \delta Q_{w,u} - h_u dm_u + \left(\sum_j h_j dm_j \right)_u \right) \quad (3)$$

$$dT_b = \frac{1}{m_b c_{p,b}} \left(V_b dp - \delta Q_{w,b} - h_b dm_b + \left(\sum_j h_j dm_j \right)_b \right) \quad (4)$$

where V_u is the unburned gases volume, V_b is the burned gases volume. The cylinder charge is supposed to be premixed and homogeneous, which implies that $dY_{i,k} = 0$.

The term $\delta Q_{th,i}$ has been replaced by $-\delta Q_{w,i}$ because the heat transfers to the surroundings are considered as heat losses into the cylinder walls. The heat losses from the gases in the combustion chamber to the cylinder walls are given by:

$$\delta Q_{w,i} = h_c A_{w,i} (T_i - T_w) \quad (5)$$

where $A_{w,i}$ is the wall transfer area for each zone, $T_i - T_w$ is the temperature difference between the gases (burned or unburned) and the cylinder walls and h_c is the heat transfer coefficient computed from Woschni's equation [12].

The volume V_i in each zone is defined by the algebraic relation:

$$V_b = \frac{m_b r_b T_b}{m_b r_b T_b + m_u r_u T_u} V_{cyl} \quad (6)$$

$$V_u = V_{cyl} - V_b \quad (7)$$

where r_i is the mixture specific gas constant in zone i and V_{cyl} is the cylinder volume. Finally, putting together equations (3) and (4) and solving for dp , the in-cylinder pressure dynamics is modeled as:

$$\begin{aligned} dp = \frac{1}{\frac{V_u}{\gamma_u} + \frac{V_b}{\gamma_b}} & \left\{ \left(1 - \frac{1}{\gamma_u}\right) \delta Q_{w,u} + \left(1 - \frac{1}{\gamma_b}\right) \delta Q_{w,b} \right. \\ & - pdV - \left(\frac{1}{\gamma_u} - 1\right) \left(\sum_j h_j dm_j\right)_u \\ & - \left(\frac{1}{\gamma_b} - 1\right) \left(\sum_j h_j dm_j\right)_b \\ & \left. + dm_u \left(\frac{1}{\gamma_u} h_u - u_u\right) + dm_b \left(\frac{1}{\gamma_b} h_b - u_b\right) \right\} \quad (8) \end{aligned}$$

COMBUSTION MODEL

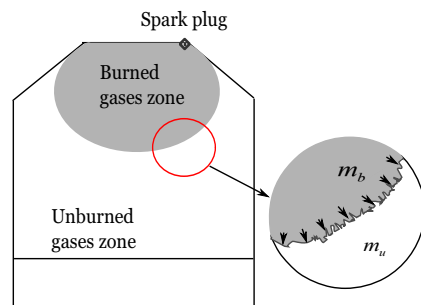


Figure 1: Two zones model scheme: the fresh gases are locally dragged to the wrinkled flame front at the laminar speed S_l

Recent combustion models are generally based on the flamelet assumption, where the combustion reaction is assumed to be fast enough so that the

dominant effect of turbulence on the flame is to wrinkle the flame surface while the inner flame structure is not significantly altered by the turbulent flow field [13]. Under these assumptions, the mass burning rate is proportional to the density of the unburned mixture ρ_u , to the turbulent flame speed S_t and to the laminar flame area A_l , considered as a spherical surface centered in the spark plug location, which implies that:

$$dm_b = \rho_u A_l S_t \quad (9)$$

After ignition, the flame surface propagates freely across the combustion chamber, the fresh gases reach the flame front at the laminar flame speed S_l and they get burned in a thin front layer. In Figure 1, a schematic view of the two zones is presented. The main idea of this model is to describe the burning rate of the fuel and the fresh air while they get burned in the combustion chamber.

The turbulent flame speed is defined as $S_t = S_l \Xi$, where S_l is the laminar speed of the flame, derived from experimental measurements in [14] as:

$$S_l = S_{L0} \left(\frac{T_u}{T_0}\right)^\alpha \left(\frac{p}{p_0}\right)^\beta (1 - 2.21 X_{egr}^{0.773}) \quad (10)$$

The parameters S_{L0} , α and β are characteristics of the fuel. In [15], specific data to characterize these parameters are given. For the study considered here:

$$\alpha = 2.4 - 0.271 \phi^{3.51} \quad (11)$$

$$\beta = -0.357 + 0.14 \phi^{2.77} \quad (12)$$

$$S_{L0} = \beta_m + \beta_\phi (\phi - \phi_m)^2 \quad (13)$$

where $\beta_m = 30.5 \text{ cm/s}$, $\phi_m = -54.9 \text{ cm/s}$ and ϕ is the equivalence ratio of the mixture.

Ξ is the turbulent wrinkling coefficient; this factor represents the increase in the flame surface, $\Xi = A_t/A_l$, where A_t is the wrinkled turbulent flame surface. Thus, the burning rate of the fuel is expressed as:

$$dm_b = \rho_u A_l S_l \Xi \quad (14)$$

During the combustion process, the wrinkling coefficient Ξ increases the turbulent burning rate. At

the beginning of the combustion the flame surface is not wrinkled by turbulence, while the flame surface reaches a given radius, it is supposed to be laminar ($\Xi = 1$). Once the transition radius is reached, the wrinkles in the upper layer of the surface are significant and this phenomenon is taken into account by the wrinkling factor that multiplies the burning rate ($\Xi > 1$).

In the literature, different ways to model this wrinkling coefficient are proposed. In this work, a fractal theory based wrinkling coefficient developed in [5] was implemented. It is detailed in the next section.

FRACTAL THEORY BASED WRINKLING COEFFICIENT

Applying fractal geometry concepts to the modeling of the wrinkled flame front surfaces has shown to give suitable estimations of the turbulent speed [16]. In the fractal model, it is assumed that the wrinkling phenomenon may be represented by a fractal dimension D_3 for a range of length scales L_{min} and L_{max} . The wrinkling coefficient Ξ is expressed as:

$$\Xi = \left(\frac{L_{max}}{L_{min}} \right)^{D_3-2} \quad (15)$$

Substituting (15) in (14) gives:

$$dm_{b_{fractal}} = \rho_u A_l S_l \left(\frac{L_{max}}{L_{min}} \right)^{D_3-2} \quad (16)$$

The fractal dimension D_3 is a function of the turbulent flow behavior inside the chamber. For this model, a simple phenomenological 0D turbulence model from [17] is retained. It is presented at the end of this document in the appendix.

The Kolmogorov's scale L_k is chosen as the minimum wrinkling scale L_{min} [5]. The maximum wrinkling scale is a function of the flame radius times a calibration constant $L_{max} = c_r R_f$, where R_f is the mean flame radius of the flame spherical surface A_l . The fractal dimension D_3 depends on the turbulence intensity u' and the laminar flame speed S_l as [5]:

$$D_3 = \frac{2.35u' + 2.05S_l}{u' + S_l} \quad (17)$$

Note that the computation of this process is assumed to start at the end of the kernel initiation process. The fractal burning rate approximation is finally obtained as:

$$dm_{b_{fractal}} = \rho_u A_l S_l \left(\frac{c_r R_f}{L_k} \right)^{D_3-2} \quad (18)$$

FLAME SURFACE

In order to implement the combustion model a well defined design of the flame surface is necessary. The flame surface model is the basis for the combustion close to the walls model. To model the combustion chamber and the flame surface progressing inside it, the following parameters are taken into account:

- cylinder geometry (Bore, spark position, chamber height);
- piston height;
- burned gases volume during combustion.

With these parameters, a simplified geometric model of the combustion chamber is obtained. The values that define this model are stored in a data map. Following the same principle, a geometric spherical surface of the flame progressing inside the combustion chamber is designed as presented in Figure 2. The data map is inverted to obtain the flame radius and the flame surface as a function of the piston height and the burned gases volume.

The input parameters to define the flame surface evolving inside the combustion chamber are the piston height and the available volume. Using the surface geometrical model and the burned gases volume from the two zones model, the input parameters of the surface model map are extrapolated during the simulation in order to obtain a flame radius and a flame surface.

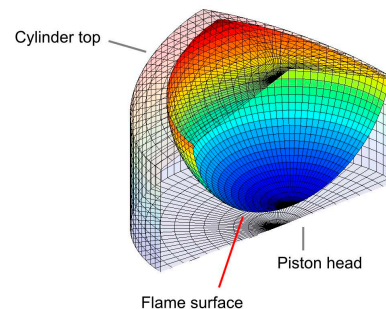


Figure 2: Scheme of the flame surface developing inside the combustion chamber

When the combustion takes place, the burned gases increase and the flame surface expands, occupying the available volume in the combustion chamber. This behavior results in changes in the burned gases density, but the burned gases volume

never decreases. In the flame surface model, the ratio between the volume of the burned gases and the available cylinder volume V_b/V_{cyl} is taken into account as an input parameter. The volumes ratio increases in time as a function of the piston height and the burned gases volume: it starts at zero at the beginning of the combustion and increases towards one, when the burned gases volume equals the available cylinder volume. This surface model is the basis to characterize the amount of flame that is close to the cylinder walls.

COMBUSTION MODEL WITH FLAME/WALLS INTERACTION

When the flame front approaches the cylinder wall, there is a deceleration of the burning rate because the boundary layer of the walls surface acts as a barrier that extinguishes the gases expansion and the relatively low temperature of the walls cools the gases. A considerable fraction of the unburned mixture actually burns in this combustion mode [18]. Consequently, the wrinkling coefficient Ξ as presented in the previous sections is valid when the flame surface propagates freely across the chamber, but the combustion close to the cylinder walls is not well represented.

Many studies have been performed in order to predict the flame-wall interaction. In [19], the flame-wall interaction is modeled by a semi-empirical expression, the Weller's approximation, but it lacks of information about its implementation. In [20] Weller's work is cited omitting the flame-wall interaction; it is replaced by a quenching law, where the burning rate near to the walls is estimated as a function of the mean burning rate and the mass fraction species (fresh gases and quenched gases). It is assumed that the quench distance is inversely proportional to the square root of the pressure. In this approximation it is not well established how to define the boundaries for the quenching zone and the estimation of the quenched gases fraction. Another approximation is proposed in [21], where the flame-wall interaction is related to the enthalpy close to the walls region, this model requires a third zone between the burned and unburned zones. In [22], a quenching coefficient is calculated measuring the length of the wrinkles in the vicinity of the piston. A linear decrease in the burning rate from a given distance to the cylinder walls was found. This result is used as an hypothesis for the final contributions of this work. This section is focused on the implementation of a submodel that represents the influence of the cylinder walls in the burning rate.

CHARACTERISTIC INTEGRAL LENGTH SCALE

A main issue to understand the flame/walls interaction is the condition where the flame surface is supposed to be influenced by the cylinder walls. As the mean flame surface is assumed to be spherical, when the

flame radius reaches a given length from the cylinder walls, the influence can be considered.

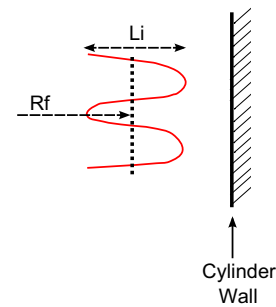


Figure 3: Scheme of the flame approaching to the cylinder walls and the distance to take into account the flame/wall interaction

In order to find the distance where the walls influence the combustion process, the fluid dynamics behavior of turbulent flows is considered. The turbulent behavior depends on the spatial distribution of the gases in the chamber and the influence of the piston movement. These characteristics are explained by the spatial and time scales of the eddy flows. The length scales are explained from 3D turbulence models, i.e [23], but 0D approximations are mainly represented by geometrical models or measurements. [24], [25] and [26] provide some estimations for the characteristic length scales .

The large scale eddies, characterized by the integral length scale L_i , represent the largest turbulent eddies occurring in a given geometry (refer to the Appendix for a more detailed explanation) as depicted in Figure 3. In this case, the integral scale seems to be a suitable reference to consider the walls influence. Thus, when the flame radius reaches a value such as $R_f > R_{cyl} - L_i/2$, the walls influence is considered.

GLOBAL APPROACH

In this section, a weighting term w that represents the transition between the turbulent combustion mode and the walls combustion mode similarly to [5] is implemented. w increases linearly with time: it models which one of the two combustion modes, fractal or near to walls, has more influence on the process. The resulting burned mass dynamics is:

$$dm_{b_{overall}} = (1 - w)dm_{b_{fractal}} + wdm_{b_{walls}} \quad (19)$$

where w is given by:

$$w = 1 - \frac{m - m_b}{(m - m_b)_{tr}} \quad (20)$$

In [5], tr is the time when the transition between the turbulent combustion mode and the walls combustion