A level-set formalism for self-ignition fronts

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1 Introduction

The level-set methods have been widely used during the past decades and have become very common to track interfaces in numerous applications as for instance image processing, robotics and fluid mechanics. The level-set approach for combustion applications has been first introduced by Williams [1] who derived the well known G-equation. In this context, the level-set function $G(\boldsymbol{x}, t)$ is a scalar field for which the iso-value G_0 corresponds to the surface that separates fresh and burned gases. This scalar field is often defined as the signed distance d to the flame front. Then, considering $G_0 = 0$ so that $G < 0$ in fresh gas and $G > 0$ in burned gas gives the following definition of the flame front: $G(\boldsymbol{x}, t) = 0$. Accordingly, differentiation of G leads to the G-equation:

$$\frac{\partial G}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} G = S_F \|\boldsymbol{\nabla} G\| \tag{1}$$

where S_F is the flame propagation speed and $\boldsymbol{u}$ the gas velocity. This G-equation is one of the fundamental tools used by the combustion community that allows for example to account for flame curvature or partially premixed mixtures. This equation has also been applied in RANS [2] as well as LES frameworks [3]. The main advantage of this method is the decoupling of the effects of the flow from the effects of the chemical reactions on the interface motion. Therefore, the Arrhenius laws involved in chemical reactions are computed preliminarily to determine the precise value of the laminar flame propagation speed S_L that is, like curvature, one of the parameters involved in S_F. This level-set strategy is perfectly suited to track flame front but cannot deal with ignition mechanisms. Accordingly, specific models are necessary to simulate most of practical reacting flows involving ignition [4] or self-ignition mechanisms. However, to the best of our knowledge, these methods have never been used to track the propagation of reaction fronts driven by self-ignition only. These mechanisms occur in gas with heterogeneous distribution of composition and temperature so that the burning zone is moving towards the unburned gases because of the variations of the ignition delay time [5]. Such self-ignition fronts have been identified in previous studies [6] as one of the leading mechanisms of the combustion process in rapid compression machines. They are also involved in the flame stabilization processes of turbulent non-premixed flames [7]. The objective of the work presented here is to propose an original level-set formalism that deals with both flame front (i.e. diffusion driven) and self-ignition front in mixtures with heterogeneous distribution of composition and temperature. Therefore, as a first step a new definition of the level-set function must be introduced to describe the displacement of self-ignition fronts.

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2 A level-set function for self-ignition fronts

In homogeneous mixtures, the self-ignition phenomenon is not a propagative mechanism but is a thermal runaway, i.e. combustion in a volume of gas, that can be described through the time evolution of the thermodynamic variables. Accordingly, the concept of front (spatial discontinuity) and its propagation is no longer valid except in heterogeneous mixtures where the time required for a mixture to ignite is variable in space. In such cases, the self-ignition delay time is a scalar field $\tau(\boldsymbol{x}, t)$ and the iso-surface defined by $\tau(\boldsymbol{x}, t) = t$ is the self-ignition front that separates fresh and burned gases. As a first step, the possible occurrence of flame front propagation after the ignition of the most reactive mixture is ignored to focus on the description of the self ignition front propagation. Then, as described in the early work of Zeldovich [5], the self-ignition front propagation speed S_I is in inverse proportion to the modulus of the gradient of self-ignition delay time:

$$S_I = \frac{1}{\|\boldsymbol{\nabla}\tau\|} \tag{2}$$

It must be noticed that molecular diffusion effects are partly taken into account via the ignition delay time $\tau(\boldsymbol{x}, t)$ that is dependent on the local thermodynamic properties submitted to diffusion. Therefore, in the context of propagation of self-ignition fronts, the G-equation becomes:

$$\frac{\partial G}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} G = \frac{\|\boldsymbol{\nabla} G\|}{\|\boldsymbol{\nabla}\tau\|} \tag{3}$$

The signed distance function is still valid and is related to time by: $G(\boldsymbol{x}, t) = (t - \tau(\boldsymbol{x}, t))\, S_I$. However, when self-ignition is involved, it may be easier to consider the level-set function H defined by $H = G/S_I$ where H is a time function:

$$\begin{cases} H(\boldsymbol{x}, t) = t - \tau(\boldsymbol{x}, t) < 0 & \text{in fresh gas} \\ H(\boldsymbol{x}, t) = t - \tau(\boldsymbol{x}, t) > 0 & \text{in burned gas} \\ H(\boldsymbol{x}, t) = 0 & \text{at the ignition front position} \end{cases} \tag{4}$$

Then, according to Equation (4), the modulus of the gradient of self-ignition delay time becomes:

$$\|\boldsymbol{\nabla}\tau\| = \|\boldsymbol{\nabla} H\| \tag{5}$$

Therefore, the H-Equations is:

$$\frac{\partial H}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} H = 1 \tag{6}$$

The H-Equation (6) is able to track self-ignition fronts and presents the advantage to be valid in homogeneous mixture when τ is constant whereas the source term of the G-Equation (3) goes to infinity in this special case. The front speed S_I is infinite in this homogeneous case but the H-function can still be used to describe the exact time of the themral runaway that occurs simultaneously throughout the volume when the value of H vanishes. It must be also noticed that the H-equation (6) is identical to the residence time transport equation that has already been used in combustion problems [8,9] but without the consideration of the level-set formalism.

Equation (3) as well as Equation (6) raises two important issues: (i) the boundary and initial conditions have a leading role so they must be prescribed with great care and, (ii) the definition of the ignition delay time $\tau(\boldsymbol{x}, t)$, i.e. its relations with local thermodynamic quantities must be clarified. The former issue is circumvented by using the normalized time function described in the next section.

3 Relevance of the normalized time function for heterogeneous mixtures

In the very simple test case where the domain is initially filled with two different gases where both of them are near ignition with $\tau_1 < \tau_2$ and perfectly segregated on each side of the plane $x_1 = 0$; the initial H-field takes two negative values associated to each gas considered:

$$H(x_1 < 0, t = 0) = -\tau_1 \qquad \text{and} \qquad H(x_1 > 0, t = 0) = -\tau_2 \tag{7}$$

Considering now the diffusion time much larger than the ignition delay times, i.e. the diffusion mechanism can be neglected, leads to a thermal runaway at $t = \tau_1$ in the most reactive mixture, i.e. for all $x_1 < 0$. Thus, as expected in this simple case, the solution of Equation (6) is exact and corresponds to $H = 0$ at $t = \tau_1$. Nevertheless, the H-equation is not related to local quantities excepted through the initial condition Equation(7). Therefore, the initial condition $H(\boldsymbol{x}, 0)$ drives the solution of Equation (6). To avoid such an issue, the level-set function is now considered as a normalized time function:

$$H^*(\boldsymbol{x}, t) = \frac{H(\boldsymbol{x}, t)}{\tau(\boldsymbol{x}, t)} \tag{8}$$

Accordingly, the gradient $\boldsymbol{\nabla} H = \tau \boldsymbol{\nabla} H^* + H^* \boldsymbol{\nabla} \tau$ reduces to $\boldsymbol{\nabla} H = \tau \boldsymbol{\nabla} H^*$ near the tracked front $H^* = 0$. Then, using Equation (5), the corresponding level-set equation writes:

$$\frac{\partial H^*}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} H^* = \frac{1}{\tau} \tag{9}$$

The initial condition with such a definition of the level-set function is $H^* = -1$ in the whole domain whatever the mixture considered. Accordingly, the solution is no more driven by the initial condition but by the ignition delay time $\tau(\boldsymbol{x}, t)$ related to local thermodynamic quantities. The goal of the next section is to validate Equation (9) for two different representative test cases.

4 Ignition in a diffusion layer

The simple test case described in the previous section, i.e. a one-dimensional diffusion layer between two different mixtures, is computed using the dilatable low-Mach DNS solver Asphodele [10]. The first set of equations is the *reference case*: it solves the sensible enthalpy and the mass fractions of chemical species using an Arrhenius law representative of a global chemical step. Unity Lewis numbers are considered for all species. The second set of equations solves is the *evaluated case*: the H^*-equation (9) associated with a non reactive scalar: the mixture fraction ξ equation (normalized total enthalpy). The self-ignition delays are preliminary computed using homogeneous reactor and stored as a function of the mixture fraction $\tau(\xi)$. In both cases, the two mixtures have the same composition but different temperatures and their mixing state are described through the use of the mixture fraction:

$$\begin{cases} \text{gas 1:} \quad \xi = 1 \quad T = 690K \quad \tau_1 = 120ms \\ \text{gas 2:} \quad \xi = 0 \quad T = 650K \quad \tau_2 = 274ms \end{cases} \tag{10}$$

Figure 1-left shows the ignition delay τ in function of ξ. The results, Figure 1-right, presents the evolution of temperature (top: *reference case*) and the evolution of the level-set function H^* (bottom: *evaluated case*) with time at the location of the most reactive mixture. The results present three different cases: (i) the negligible diffusion case (red curve), i.e. the two mixtures stay perfectly segregated and ignition occurs at $t = \tau_1$, (ii) the infinitely large diffusion case (blue curve), i.e. an homogeneous mixture is obtained

instantaneously at $\xi = 0.5825$ and (iii) the stratified case where ignition occurs during the mixing process (black line). As expected, the results are exact in the two limit cases, i.e. red and blue curves and, indeed, are also excellent in the stratified case. In the former cases (red and blue curves) the straight lines obtained show that the ignition delay time as well as the mixture fraction are constant during the computations. In the latter case (black), the H^* growth initially corresponds to the perfectly segregated case for $t < 40ms$ (red) and progressively diverges as the two gases mix. Eventually, the level-set function vanishes ($H^* = 0$) at the same time as the thermal runaway (see Figure 1-top-right: reference case).

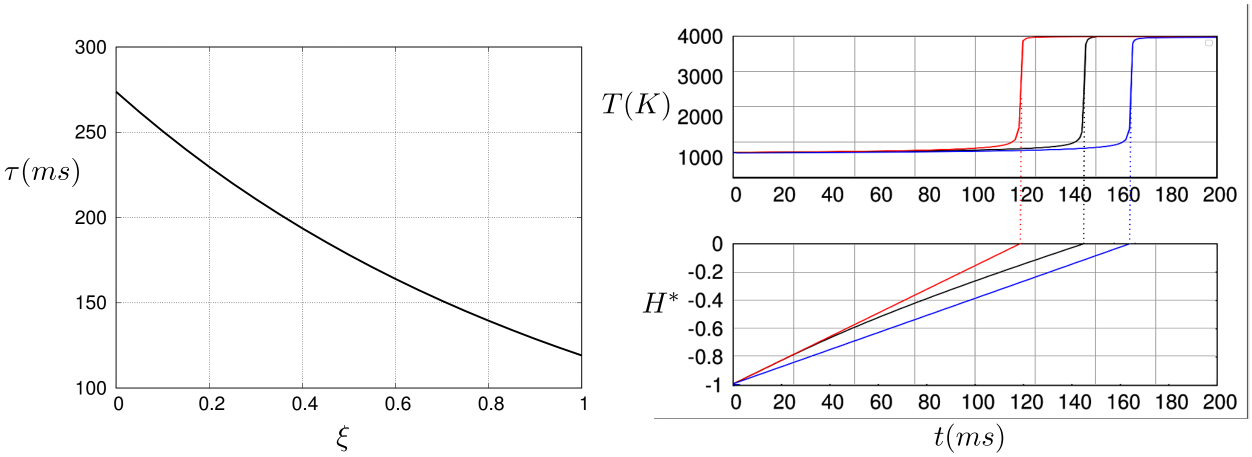

Figure 1: Left: Ignition delay time versus mixture fraction $\tau(\xi)$, Top-Right: Temperature profile versus time obtained with an Arrhenius law, Bottom-Right: Level set function H^* versus time. Red curves: negligible diffusion, blue curves: infinitely large diffusion, black curves: stratified conditions

5 Ignition of an homogeneous mixture submitted to compression

Another representative test case corresponds to a rapid compression of an homogeneous mixture where the self-ignition delay time has the same order of magnitude as the compression time. This case corresponds to an experiment carried out with the rapid compression machine of Pprime Institute [6] where chemical reactions begin before the end of compression. Then, the ignition delay time is not representative of any given state but is the result of the successive gas conditions (pressure and temperature) obtained during the compression. Accordingly, the ignition delay times $\tau(t)$ ($0D$ simulations are considered here) resulting from these fresh conditions during the compression are preliminarily computed using a detailed chemical mechanism and stored as a function of the fresh gas T_u. Figure 2-left shows the ignition delay time for the largest values of the fresh gas temperature. Figure 2-top-right shows the temperature versus time obtained using a detailed chemical mechanism (*reference case*) and Figure 2-bottom-right shows the solution of Equation (9) (*evaluated case*). The ignition time obtained using the level-set function, i.e. $H^* = 0$, perfectly matches the detailed chemistry result. The H^* profile is flat at the beginning, i.e. $\tau \to \infty$, and then progressively increases during the compression for finite values of the ignition delay time. Eventually, a straight line is obtained after the end of the compression when the ignition delay time becomes constant.

The results of these two test cases show the relevance of the level-set strategy based on the normalized time function to model the self-ignition process in heterogeneous mixtures. This level-set method avoids the appearance of the strong non-linearities induced by the use of Arrhenius laws but takes their effects into account via the tabulated ignition delay time.

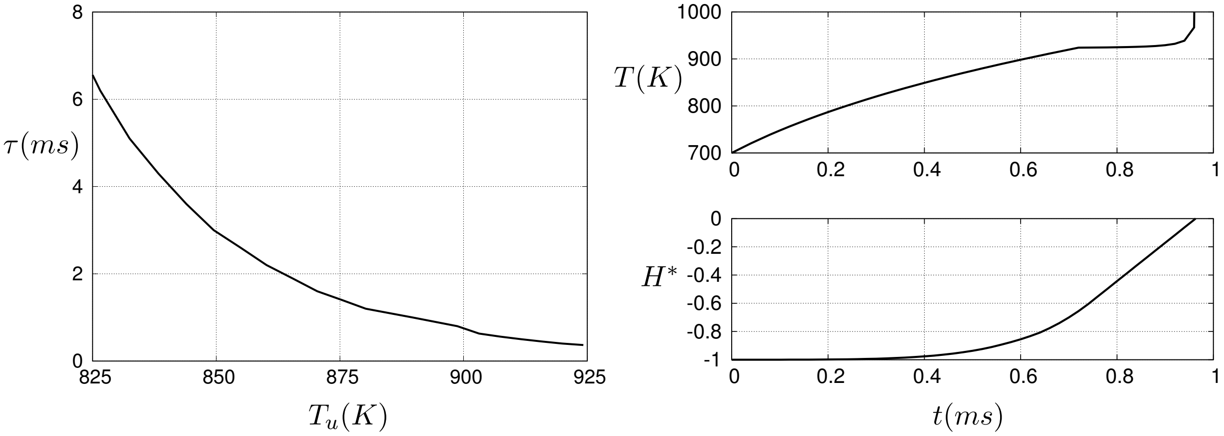

Figure 2: Left: Ignition delay time versus temperature of fresh gas $\tau(T_u)$, Top-Right: Temperature profile versus time obtained using a detailed chemical mechanism, Bottom-Right: Level set function H^* versus time.

6 Conclusions and perspectives

This work provides an original level-set formalism. This formalism and the corresponding equation is validated in two cases: ignition in a diffusion layer and ignition of an homogeneous mixture submitted to compression. The new definition of the level-set function introduced in this work involves a normalized time that accounts for local effects on the ignition process. The solving of the equation for the normalized time function H^* provides accurate values of the self ignition times in situations where diffusion or compression effects must be taken into account. The complete validation of the moving front inside the diffusion layer is a work in progress and the limits of this strategy must also be further analyzed with 3D direct numerical simulations. This strategy has also been extended to account for self-ignition/flame fronts interactions and applied to the Large Eddy Simulation of a constant volume combustion chamber available at Pprime Institute [11]. Figure 3 shows preliminary results that correspond to the flame front computed with Open-Foam. A self-ignition kernel appears and grows (two first snapshots on the left side of Figure 3) by mixing between fresh and hot residual burned gas and eventually transits to a flame front.

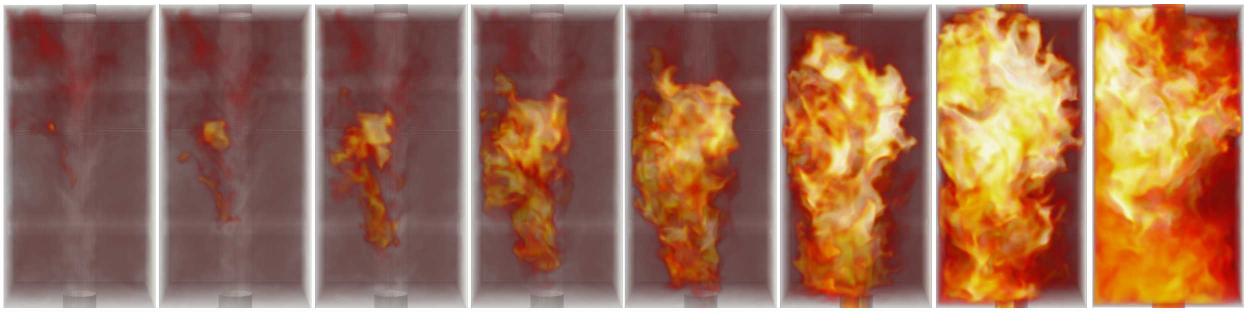

Figure 3: Large Eddy Simulation of a constant volume combustion chamber using the H^* equation. Temperature field of a self-ignited cycle [11]

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