A level-set transport equation for tracking self-ignition fronts in hydrogen-air mixture

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1 Introduction

In the context of energy transition, one of the possible solutions to gradually reduce the release of fossil carbon into the atmosphere is to progressively increase the proportion of hydrogen or biofuels and reduce that of conventional fuels used in combustion systems, as engines or gas turbines. The fuel mixture will therefore be even more heterogeneous. The combustion process in presence of large spatial temperature and composition variations may lead to unexpected physical mechanisms as self-ignition front propagation. Then, the detailed understanding of such reactive heterogeneous flows remains essential for the design of more clean and efficient combustion systems. The self-ignition and flame propagation interactions occurring in these heterogeneous mixtures has been extensively studied over the past decades [1, 2] and still produce an abundant literature [3–6]. However, most of the existing turbulent combustion models are no more valid to describe the propagation of flames through such heterogeneous mixtures where the occurrence of transition from diffusive to self-ignition propagation modes is highly probable. Such mechanisms and their interactions are responsible for local flame accelerations and may lead to the destruction of practical systems. In this context, new models must be proposed and implemented in computational tools to simulate the main behavior of flows but also to anticipate the possible occurrence of rare events responsible of industrial accidents.

The objective of this work is to develop and validate a new model dealing with transitions from self-ignition to flame propagation. The use of a detailed chemical scheme provides computational results of these transitions in sufficiently good agreement with observations when the mesh resolution is high enough to deal with Arrhenius laws. However, for multidimensional simulations, the very high computational power required to obtain both realistic self-ignition times and flame propagation speed constitute a serious limitation to the generalization of this approach. Therefore, the strategy considered here relies on a tabulation method where both homogeneous reactors and one-dimensional flames are computed preliminary using detailed chemical schemes [7]. Then, the most important reactive properties, as self-ignition times and flame propagation speed, are stored as functions of a reduced set of variables to be re-used in multi-dimensional simulations of practical turbulent flows. This abstract focuses on the validation using DNS of the most original proposition of this strategy: a level-set transport equation to track the propagation of self-ignition fronts [8].

Self-ignition fronts appear in gas with heterogeneous distribution of composition and temperature so that the burning zone is apparently moving towards the fresh gases because of the variations of the local self-ignition time [9]. Thus, a level-set function similar to the one introduced for combustion applications by Williams [10] can be defined to locate the self-ignition front. However, this new level-set function represents a time field instead of a distance field. Its definition comes from the comparison

of the residence time field with the local ignition delay time. The level-set equation proposed appears to be equivalent to the normalized residence time equation recently introduced by Wang et al. [7]. The validation cases presented here are a 1D diffusion layer and a 2D heterogeneous flow representative of the mixing of two hot hydrogen-air mixture. The simulations are performed with the DNS code Asphodele [11] which is a multispecies low-Mach solver. The reference results are obtained by considering the detailed chemical mechanism of Ó Conaire et al [12]. The initial conditions of temperature are set to analyze the effect of the diffusion mechanism on the ignition time of the mixture. The level-set function field results in a clear identification of the leading physical mechanism of the front propagation: either self-ignition or laminar flame.

2   The level-set transport equation for self-ignition fronts

The self-ignition phenomenon is a thermal runaway that can be described in homogeneous reactors through the time evolution of the thermodynamic variables, see the temperature profile of Figure 1 left. In heterogeneous mixtures, the time required for a mixture to ignite is variable in space: the self-
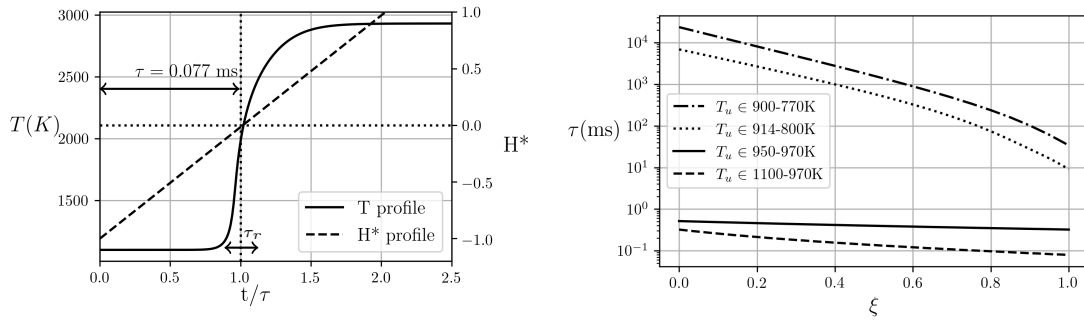
Figure 1: Evolution versus time of T and H* in a homogeneous reactor (left). Ignition time τ versus ξ (right) for four different ranges of initial fresh gas temperature T_u.

ignition delay time is a scalar field $\tau(\boldsymbol{x}, t)$. As the characteristic burning time τ_r, see Figure 1 left, is much smaller than the ignition time, the chemical reactions are located in a small zone between fresh and burned gases. Thus, the iso-surface defined by $\tau(\boldsymbol{x}, t) = t$ is the self-ignition front. Then, as described in the early work of Zeldovich [9], the self-ignition front propagation speed S_I is in inverse proportion to the modulus of the gradient of self-ignition delay time:

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

The introduction of this propagation speed in the well known G-equation [10] gives a transport equation to track self-ignition front where G is the signed distance to the front:

$$\frac{\partial G}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} G = S_I \|\boldsymbol{\nabla} G\| \tag{2}$$

However, solving Eq. (2) presents different difficulties related to the definition of the boundary and initial conditions of G for fully fresh gases conditions. Accordingly, another definition of the level-set function and a change-of-variable are necessary. First, the time function $H(\boldsymbol{x}, t) = t - \tau(\boldsymbol{x}, t)$ is the new level set function and combining Eq. (1) and (2) gives:

$$\frac{\partial H}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} H = 1 \tag{3}$$

Then, H is normalized: $H^*(x,t) = H(x,t)/\tau(x,t)$ so that its equation writes:

$$\frac{\partial H^*}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} H^* = \frac{1}{\tau} - \frac{H^*}{\tau} \left(\frac{\partial \tau}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} (\tau) \right) \tag{4}$$

Then, for the sake of simplicity, the last term of the right-hand-side of Eq. (4) is modeled as a diffusion term for H^*. The H^*-equation and associated initial condition writes:

$$\frac{\partial H^*}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} H^* = D \triangle H^* + \frac{1}{\tau} \qquad H^*(t=0) = -1 \quad \forall \, \boldsymbol{x} \tag{5}$$

The definition of the initial and boundary values for fresh gases conditions does not present any more difficulty: $H^* = -1$. It is important to note that Equation (3) is equivalent to the residence time transport equation [13] and Eq. (5) is equivalent to the normalized resident time equation introduced in [7]. Figure 1 left shows the evolution of H^* obtained solving Eq. (5) in an homogeneous reactor. The solution is exact in this simple 0D case: H^* vanishes and the heat release reaches a maximum simultaneously.

3   Initial conditions and characteristic times

For the 1D and 2D cases, the computational domains are initially filled with fresh gases corresponding to stoichiometric hydrogen/air mixtures at two different temperatures. Accordingly, a mixture fraction ξ is introduced as follow: $\xi = (h - h_l)(h_h - h_l)$, where h is the gas enthalpy and h_h, h_l are the corresponding extreme values used as intitial conditions. Four ranges of initial enthalpy $h \in [h_l, h_h]$ has been considered. Figure 1 right shows the ignition delay times as functions of mixture fractions $\tau(\xi)$ corresponding to these ranges. The ξ-fields are initially highly segregated both in 1D and 2D cases, see Figure 2 left and middle. The domain is $0.01m$ in each direction and each composed of 128 cells. For the 2D cases, the initial fields of temperature and mixture fraction are generated with the procedure from Bouali et al [5], see Figure 2 middle.
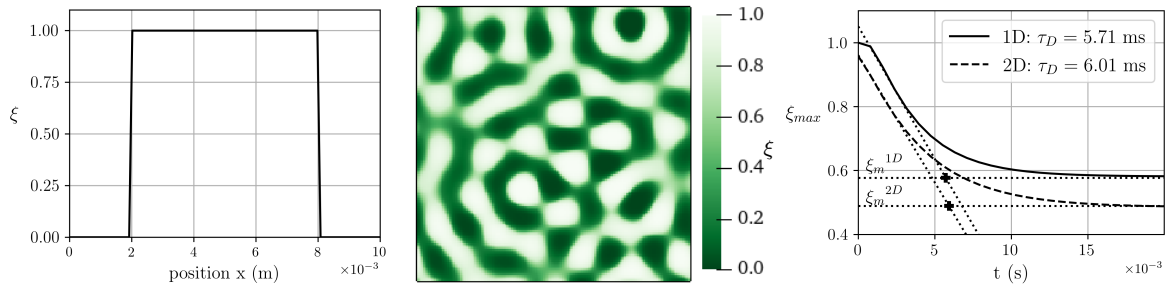

Figure 2: Initial ξ-fields for 1D case (left) and 2D case (middle). Time evolution of the maximum value of mixture fraction in the 1D and 2D domains.

As our objective is to analyze the interaction between self-ignition and diffusion mechanisms, the characteristic diffusion time τ_D must be introduced. Figure 2 right shows time evolution of the maximum value of the mixture fraction reached in the domain for two non reactive computations corresponding to 1D and 2D cases with similar diffusion times. The mixture fraction value reaches $\xi = \xi_m$ when the mixture becomes homogeneous. The crosses in Figure 2 right corresponds to the definition of the characteristic diffusion time τ_D considered in this study. Then, the following non dimensional numbers are introduced:

$$R_h = \frac{\tau_D}{\tau_h} \quad \text{and} \quad R_l = \frac{\tau_D}{\tau_l} \quad \text{and} \quad R = \frac{R_l}{R_h} = \frac{\tau_h}{\tau_l} \tag{6}$$

where τ_h and τ_l are the extreme values of self-ignition delay times corresponding respectively to $\xi = 1$ and $\xi = 0$. The R-value is lower than unity and vanishes when the self-ignition times strongly varies in space. The R_h-value vanishes when the mixing mechanism is faster than the self-ignition of the most-reactive mixture and R_h is large when molecular diffusion is negligible. The values of the non dimensional numbers corresponding to the 1D-simulations and 2D-simulations performed are gathered in Table 1.

Table 1: Gas conditions retained for 1D and 2D simulations

Cases	1D-1	1D-2	1D-3	2D-1	2D-2	2D-3
R	1.4×10^{-3}	1.4×10^{-3}	0.2	1.4×10^{-3}	0.65	0.2
R_h	$0.2 \rightarrow 100$	$0.2 \rightarrow 100$	$0.5 \rightarrow 100$	$0.5 \rightarrow 100$	$0.5 \rightarrow 100$	$0.5 \rightarrow 10000$
T_h (K)	900	914	1100	900	970	1100
T_m (K)	845	866	1045	845	961	1045
T_l (K)	770	800	970	770	950	970
τ_h (s)	3.49×10^{-2}	9.2×10^{-3}	7.89×10^{-5}	3.49×10^{-2}	3.23×10^{-4}	7.89×10^{-5}
τ_m (s)	9.63×10^{-1}	3.48×10^{-1}	1.22×10^{-4}	9.63×10^{-1}	3.85×10^{-4}	1.22×10^{-4}
τ_l (s)	$2.36 \times 10^{+1}$	6.88×10^{0}	3.23×10^{-4}	$2.36 \times 10^{+1}$	4.98×10^{-4}	3.23×10^{-4}

4   Results

Figure 3 shows the time evolution of the maximum of temperature, i.e. at the center of the 1D domain, for two R-values and three R_h-values. The boundary profiles, i.e. $R_h >> 1$ and $R_h << 1$, correspond to the limit cases where homogeneous conditions respectively for $\xi = 1$ and $\xi = \xi_m$ are set initially. Accordingly, intermediate values of R_h corresponds to cases where the mixing mechanism affects the self-ignition time of the most reactive mixture but the gases are still heterogeneous in the domain. The minimum value of the self-ignition time obtained, i.e $R_h >> 1$, is two times smaller than the maximum value, i.e. $R_h << 1$, for $R = 0.2$ but hundred times smaller for $R = 1.4 \times 10^{-3}$. These simple computations therefore allow to study a wide spectrum of self-ignition/mixing interactions. Figure 4
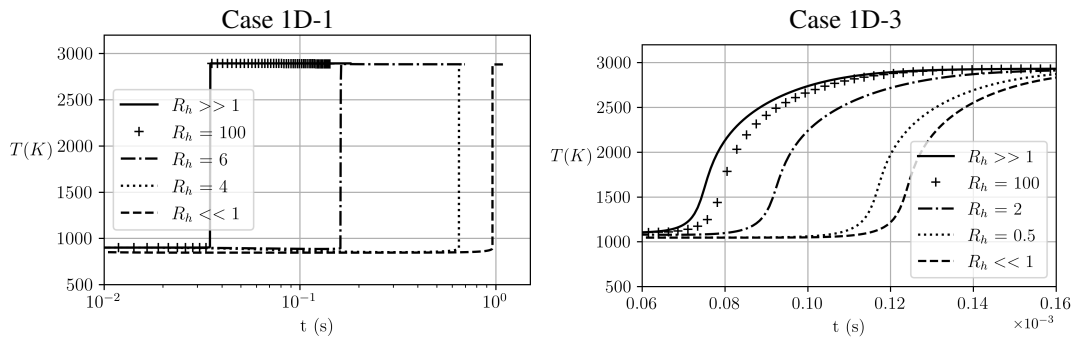

Figure 3: Time evolution of the maximum value of temperature in the 1D domain for different values of R_h and $R = 1.4 * 10^{-3}$ (left) and $R = 0.2$ (right). The left time-axis is a log-scale

shows similar profiles of Figure 3 but using a normalized time-scale. It also displays the H^*-profile obtained from Eq. 5. The value of H^*, initially set to -1, vanishes at the ignition time whatever the case considered. This result proves that the use of the function $\tau(\xi)$ in association with Eq. 5 allows the precise evaluation of the self-ignition time in a gas subjected to a mixing process whatever the value of R_h. It is also important to notice that the H^*-profile for $R_h = 4$ displays a non linear shape due to the

strong diffusion mechanism (large variation of local ignition delay time) during the ignition process. In this case, the temperature of the most reactive mixture decreases before ignition occurs, see Figure 4 left. Moreover, as the source term of Eq. 5 cannot be negative, the decrease of H^* observed for $R_h = 4$, is the signature of the modeled diffusion term. This result clearly shows the importance of the diffusion term in H^* to obtain the right ignition time when the order of magnitude of the characteristic diffusion and self-ignition times are the same (R_h is order unity). This mechanism rejuvenates particles close to self-ignition by mixing with younger (fresher) particles.
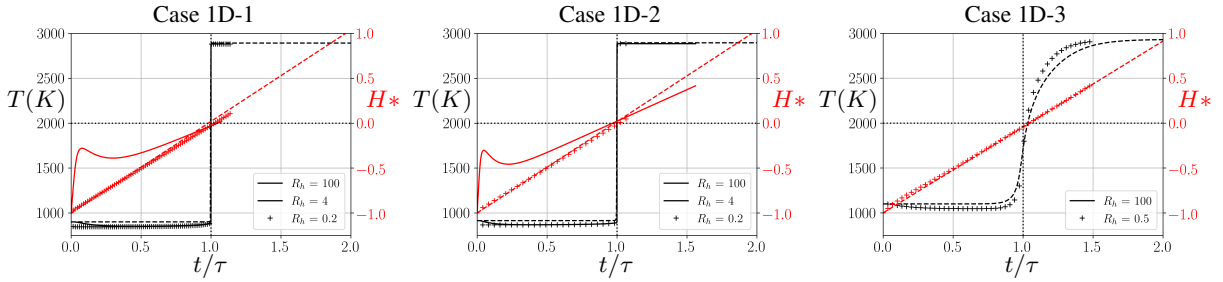

Figure 4: Time evolution of the temperature and H^* of the most reactive mixture, i.e. at the center the 1D domain for three values of R and different values of R_H.

Finally, the 2D cases Fig. 5-left) provide similar results: the H^*-field vanishes and the heat release reaches a maximum simultaneously and at the same location, i.e. in the most reactive mixture ($\xi = 1$). Figure 5 also presents isocontours of $H^* = 0$ (blue) and isocontours of maximum values of heat
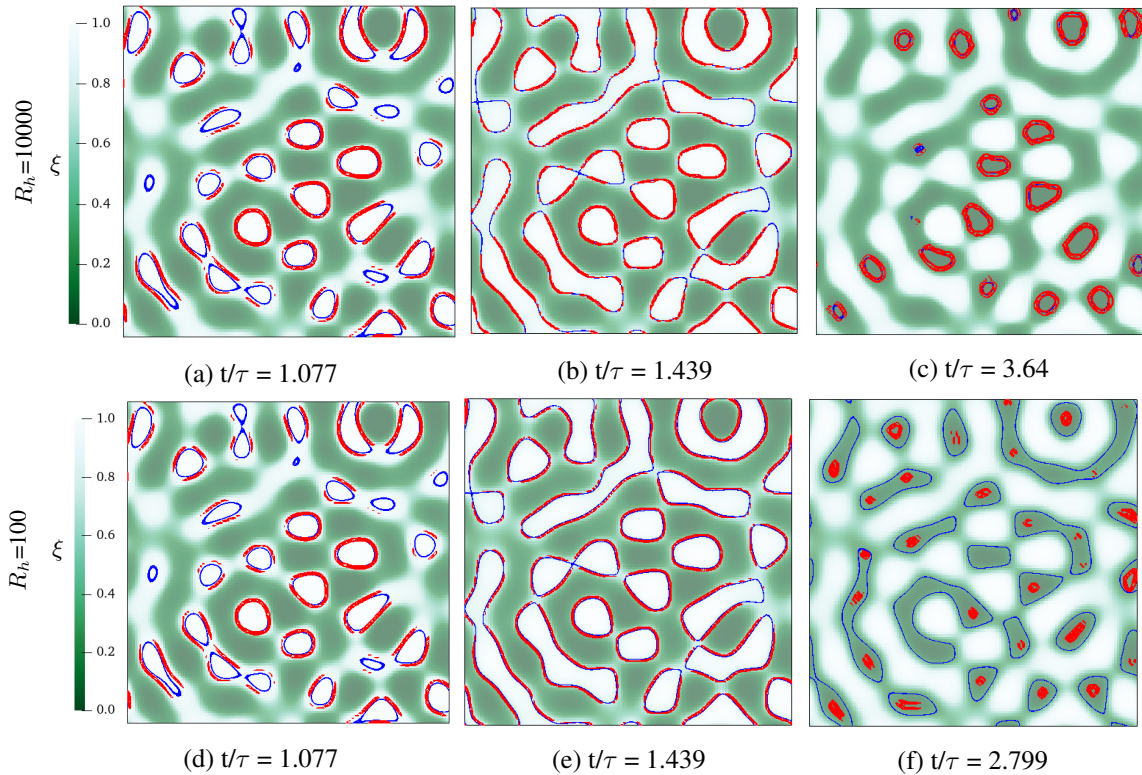

Figure 5: Temperature iso-contour for case 2D-3 and $R_h = 10000$ (Top) and $R_h = 100$ (Bottom) at different time steps. The physical time is normalized with the self-ignition time of the most reactive mixture

release (red) at three times steps after self ignition of the most reactive mixture. The reactive front are propagating from regions of high ξ-values to low ξ-values. The red and blue isocontours perfectly coincide during the whole combustion process for $R_h = 10000$, see the Sub-figures (a) (b) and (c). However, for $R_h = 100$, the $H^* = 0$-isocontours and isocontours of maximum heat release diverge before the end of the combustion process, see the sub-figures (f). This separation of isocontours is characteristic of a transition from a self-ignition front to a laminar flame propagation.

Eventually, these results highlight the relevance of the level-set approach based on the H^*-equation to track the self ignition fronts in the presence of a significant diffusion process. The resulting H^*-field also yields a clear identification of the transition between self-ignition and laminar flame propagation.

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