Characterization of differential diffusion effects during the constant volume ignition of a temperature stratified lean premixed hydrogen/air mixture subject to decaying turbulence

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Chen and coworkers recently performed a Direct Numerical Simulation (DNS) of the constant volume ignition of a very lean hydrogen/air subject to different levels of temperature stratification [E. R. Hawkes, R. Sankaran, P. P. Pèbay, J. H. Chen, Combustion and Flame 145(1-2):145-159]. Under high levels of temperature stratification, two distinct modes of combustion are found: deflagrations and spontaneous ignition fronts. Deflagrations propagate in regions of high temperature gradient and low flame front curvature, while spontaneous ignition is associated with highly curved, low temperature gradient fronts. The simulations included hydrogen/air finite rate chemistry and molecular transport based on a Lewis number formulation for individual species. Differential diffusion effects are present for all temperature stratification cases and they become more pronounced as the level of stratification increases. At the highest level of temperature stratification tested, we find that differential diffusion has an impact on the overall heat release rate. By comparing simulations with and without differential diffusion, we find that differential diffusion has a twofold effect on the ignition event. Early in the ignition, regions with a hydrogen mass fraction higher than the nominal levels are created and they subsequently burn to achieve higher temperatures, which can be accounted for by simple equilibrium calculations. Later in the ignition process, differential diffusion enhances heat release rate in regions of high curvature where deflagrations are present, as generally expected in lean hydrogen/air premixed flames.

1 Introduction

Hydrogen is expected to play an increasingly important role among fuels for automotive applications, given its CO\textsubscript{2} free nature and excellent combustion characteristics. Recent research efforts focused on the usage of hydrogen in Homogeneous Charge Compression Ignition (HCCI) engines, either as an engine fuel [1] or in a mixture with other fuels [2]. Experimental evidence suggests that hydrogen can be used as a primary fuel for HCCI engines, albeit in a very lean mixture (0.1 < Φ < 0.3) due to hydrogen’s very fast burning characteristics and high heat release rate. When used as an additive, it was found that hydrogen stabilizes combustion in a natural gas
HCCI engine in various difficult combustion conditions. Also, hydrogen and carbon monoxide are products of catalytic reformation of several alcohol fuels (e.g. methanol), which are currently put forward as viable HCCI fuels. Hydrogen’s ignition and combustion characteristics are markedly different from hydrocarbons such as methane, ethane, propane, butane and similar. The most salient characteristics are that the minimum ignition energy of hydrogen is very low, its laminar flame speed is greater than gaseous hydrocarbons and its flammability limits are wider [3]. Furthermore, hydrogen has a very high diffusivity coefficient, which results in its differential diffusion, possibly altering combustion macro characteristics such as heat release rate, turbulent flame speed and burning rate [4]. The limited experience in the field of hydrogen turbulent combustion under HCCI-like conditions is an obstacle to the development of engineering models. The modeling of ignition in a HCCI engine poses several challenges in itself, mainly due to the presence of temperature and mixture inhomogeneities. For example, the presence of Exhaust Gas Recirculation (EGR) [5], the extent of turbulent mixing [6, 7], and heat losses to the walls [8] can cause the temperature and/or the composition to be inhomogeneous. Chen et al. [9] and Hawkes et al. [10] have shown that under increasing temperature stratification a mixed combustion mode is present during the ignition of a lean hydrogen/air mixture at HCCI-like conditions. Combustion occurs both as spontaneous ignition as well as deflagration. In this work, we study the occurrence of differential diffusion in the ignition of a lean hydrogen/air mixture subject to different levels of temperature stratification (see Ref. [9]). We present a transport equation for the mixture fraction defined on the mass fraction of the hydrogen atom. For each level of temperature stratification we study the dynamics of differential diffusion as well as the impact of differential diffusion on the global and local heat release rates. Further discussion is made on the statistics of the stretch (both tangential and curvature components) and their impact on the burning rate and occurrence of differential diffusion.

2 Numerical method

The DNS data pertains to the ignition of a lean (equivalence ratio $\Phi = 0.1$) charge of hydrogen and air at conditions similar to those in a HCCI engine cylinder near Top Dead Center (TDC) at the end of the compression stroke (geometric compression ratio is 15:1). The DNS domain is two-dimensional and it extends 4.1 mm in each direction with periodic boundary conditions. Also, the simulation is carried out in such a manner that background pressure increases as a result of a constant volume constraint. Hence, compression heating as a result of igniting kernels is an integral part of the simulation. The compression stroke (not modeled) elevates the pressure and temperature from 1 atm to 41 atm and from 400 K to 1070 K respectively. The velocity flow field is initialized with homogeneous, isotropic turbulence, which is then allowed to decay during the simulation. Random temperature fluctuations of given magnitude are imposed on the temperature field and a parametric study is performed by varying the root-mean-square (r.m.s.) of the stratification. Four cases were considered in the DNS study with r.m.s. of the temperature at: 3.75 K, 7.5 K, 15 K and 30 K. However, in this work we will focus our attention on the cases of 3.75, 15 and 30 K, which we name cases A, B, and C. Additionally, the cases with r.m.s. 15 and 30 K have also been computed with a unity Lewis number formulation (cases D and E). All cases are summarized in Table 1 and additional details of the DNS methodology, configuration and parameters can be found in [9, 10]. Important turbulence parameters include the turbulence intensity $u'$, the integral length
Table 1: List of all DNS parametric studies. See also Refs. [9,10] for additional details.

<table>
<thead>
<tr>
<th>Case</th>
<th>$T_{r.m.s.}$ (K)</th>
<th>Note</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>3.75</td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>15.0</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>30.0</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>15.0 Le = 1</td>
<td></td>
</tr>
<tr>
<td>E</td>
<td>30.0 Le = 1</td>
<td></td>
</tr>
</tbody>
</table>

Table 2: List of length, time and velocity scales along with non dimensional parameters. Laminar flame data from PREMIX [11].

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u'$ (m/s)</td>
<td>0.5</td>
</tr>
<tr>
<td>$L_{11}$ (mm)</td>
<td>0.34</td>
</tr>
<tr>
<td>$L_{ue}$ (mm)</td>
<td>1.0</td>
</tr>
<tr>
<td>$\tau_t$ (ms)</td>
<td>0.68</td>
</tr>
<tr>
<td>$\delta_F$ (mm)</td>
<td>0.47</td>
</tr>
<tr>
<td>$S_L$ (m/s)</td>
<td>0.65</td>
</tr>
<tr>
<td>$\tau_F$ (ms)</td>
<td>0.72</td>
</tr>
<tr>
<td>$u'/S_L$</td>
<td>0.77</td>
</tr>
<tr>
<td>$L_{11}/\delta_F$</td>
<td>0.72</td>
</tr>
<tr>
<td>$\tau_t/\tau_F$</td>
<td>0.94</td>
</tr>
</tbody>
</table>

scale computed from a two-point correlation $L_{11}$, the most energetic turbulence length scale $L_{ue}$ and the eddy turnover time $\tau_t = L_{11}/u'$. Other scales of interest are the (unstrained) laminar flame speed $S_L$ computed for $\Phi = 0.1$ at 41 atm and 1070 K, the flame thermal thickness $\delta_F$ defined as in Eq. (1) and the flame time $\tau_F = \delta_F/S_L$.

$$\delta_F = \frac{T_b - T_u}{dT/dx|_{max}}$$  \hspace{1cm} (1)

where the subscripts $u$ and $b$ correspond to the unburnt and burnt states respectively. The thermal diffusivity of the mixture $D_{th}$ is computed as a function of temperature ($\propto T^{0.7}$) density [12], while the mass diffusion coefficients for individual species are computed by constant Lewis numbers given in Table 3 as $D_i = D_{th}/Le_i$.

3 Mixture fraction definitions

Mixture fraction is a concept customarily used to describe mixing of fuel and oxidizer in non-premixed flames. However, we find such concept useful in this study to identify the occurrence of localized differential diffusion. Note that the computational domain is initialized with a mixture with constant composition. As such, deviations from the initial value of the proportions of fuel and oxidizer indicate differential diffusion. Let us now introduce several definitions of mixture fraction. The element-based mixture fraction is defined as $\xi_e$

$$\xi_e = \xi_e(Z_e) = \frac{Z_{e,2} - Z_{e,1}}{Z_{e,2} - Z_{e,1}}$$  \hspace{1cm} (2)

where $Z_e$ is the element-based local mass fraction of element $e$ and subscripts 1 and 2 refer to the fuel and oxidizer streams respectively. The mixture fraction $\xi$ for a hydrogen-oxygen system is defined according to [13] as

$$\xi = \frac{\xi_O + \alpha \xi_H}{1 + \alpha}$$  \hspace{1cm} (3)

3
Table 3: Lewis number used for diffusive transport for each species alongside with several other coefficients used in the definition of a transport equation for $\xi_H$.

<table>
<thead>
<tr>
<th>Species</th>
<th>Lewis Nr</th>
<th>$\beta_i$</th>
<th>$\gamma_i$</th>
<th>$\delta_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_2$</td>
<td>0.30</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$O_2$</td>
<td>1.11</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
</tr>
<tr>
<td>$O$</td>
<td>0.70</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
</tr>
<tr>
<td>OH</td>
<td>0.73</td>
<td>0.054</td>
<td>-1.94</td>
<td>-0.116</td>
</tr>
<tr>
<td>$H_2O$</td>
<td>0.83</td>
<td>0.1121</td>
<td>-2.12</td>
<td>-0.238</td>
</tr>
<tr>
<td>$H$</td>
<td>0.18</td>
<td>1.0</td>
<td>2.22</td>
<td>2.222</td>
</tr>
<tr>
<td>$HO_2$</td>
<td>1.10</td>
<td>0.0306</td>
<td>-2.42</td>
<td>-0.074</td>
</tr>
<tr>
<td>$H_2O_2$</td>
<td>1.12</td>
<td>0.0594</td>
<td>-2.44</td>
<td>-0.145</td>
</tr>
<tr>
<td>$N_2$</td>
<td>1.04</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
</tr>
</tbody>
</table>

where $\alpha = \nu_H (Z_{H,1} - Z_{H,2})/(Z_{O,2} - Z_{O,1})$, and $\nu_H = W_O/(2W_H)$, with $W_O = 15.999$ g/mol and $W_H = 1.008$ g/mol being the atomic weights of O and H. In the present work, the two elements are H and O, and $Z_{H,1} = 1$, $Z_{H,2} = 0$, while $Z_{O,1} = 0$ and $Z_{O,2} = 0.233$. Equation (2) then reduces to

$$\xi_H = Z_H$$

(4)

$$\xi_O = 1 - \frac{Z_O}{Z_{O,2}}$$

(5)

The mixture fraction at the onset of the simulation, either defined based on elements (H or O) according to (2) or (3), are identical and equal to $\xi_0 = 2.927 \times 10^{-3}$ throughout the flow field, which corresponds to an equivalence ratio of $\Phi = 0.1$ according to the following

$$\Phi = \frac{\xi/(1 - \xi)}{FA_{stoi}}$$

(6)

where $FA_{stoi} = 0.02936$ is the fuel ($H_2$) to oxidizer (air at 21% vol $O_2$) mass ratio for a stoichiometric hydrogen-air mixture. Here we chose to characterize differential diffusion using $\xi_H$ as opposed to $\xi_H - \xi_O$ as in other works [14], since the mixture is premixed and lean, with hydrogen being the only fuel component so that $\xi_H = Z_H$. A value of $\xi_H$ in excess of the base value of $\xi_0 = 2.927 \times 10^{-3}$ indicates a pocket of mixture which has a higher fuel content and once fully burnt achieves a higher temperature.

Starting from the definition of $\xi_H = Z_H$ we can write a transport equation for the H atom based mixture fraction as

$$Z_H = Y_{H_2} + Y_H + \beta_{OH} Y_{OH} + \beta_{H_2O} Y_{H_2O} + \beta_{HO_2} Y_{HO_2} + \beta_{H_2O_2} Y_{H_2O_2}$$

(7)

where $Y_i$ are the species mass fractions and $\beta_i$ are the H atom mass fraction in molecule $i$ which we report in Table 3. From Eq. (7) and Table 3 is obvious that the mass fractions of $H_2$, $H$ and $H_2O$ play the greatest parts in defining the overall H-atom mixture fraction $\xi_H$. Let us first assume that the quantity $\rho D_i$ is approximatively constant for all species. Then recall that the transport equation for a species mass fraction in a reactive flow can be written as

$$\frac{\partial Y_i}{\partial t} + \mathbf{u} \cdot \nabla Y_i = D_i \nabla^2 Y_i + \frac{\dot{\omega}_i}{\rho}$$

(8)
where $\dot{\omega}_i$ is the mass source term per unit volume of species $i$, $D_i = D_{th}/Le_i$, with $Le_i$ being the Lewis number of species $i$ as in Table 3 and $D_{th}$ is the thermal diffusivity of the mixture. In view of the large nitrogen dilution in the mixture, we expect Fick’s law to be accurate enough for the purposes of our analysis. Now take the time derivative on both sides of Eq. (7), substitute Eq. (8) and group terms to obtain

$$\frac{\partial \xi_H}{\partial t} + \mathbf{u} \cdot \nabla \xi_H = D_{H_2} \nabla^2 \xi_H + \beta_{H_2O} (D_{H_2O} - D_{H_2}) \nabla^2 Y_{H_2O} + \beta_{H_2O_2} (D_{H_2O_2} - D_{H_2}) \nabla^2 Y_{H_2O_2} + \beta_{HO_2} (D_{HO_2} - D_{H_2}) \nabla^2 Y_{HO_2}$$

Interestingly, Eq. (9) indicates that sources of $\xi_H$ are connected to the Laplacian of mass fractions of products (H$_2$O) or intermediates of combustion (H, OH, H$_2$O$_2$, and HO$_2$), thus stressing the importance of chemical reactions in driving differential diffusion. The term $\nabla^2 \xi_H$ represents diffusion of fuel mass fraction. The terms in Eq. (9) can be rewritten in a manner that makes explicit the different contributions of the species. Each term $D_i - D_{H_2}$ is rewritten as $D_{th}(1/Le_i - 1/Le_{H_2}) = D_{th}\gamma_i$, where $\gamma_i$ are defined in Table 3. Then Eq. (9) becomes

$$\frac{D\xi_H}{Dt} = \frac{D_{th}}{Le_{H_2}} \nabla^2 \xi_H + D_{th}\delta_{H_2O} \nabla^2 Y_{H_2O} + D_{th} \left[ \delta_H \nabla^2 Y_H + \delta_{OH} \nabla^2 Y_{OH} \right] + D_{th} \left[ \delta_{H_2O_2} \nabla^2 Y_{H_2O_2} + \delta_{HO_2} \nabla^2 Y_{HO_2} \right]$$

$$= (D_{th}/Le_{H_2}) \nabla^2 \xi_H + \Omega_p + \Omega_r$$  \hspace{1cm} (10)

where we redefined the $\delta_i$ factors explicitly in Table 3 and we indicated with $\Omega_p$ the mixture fraction source due to chemical reactions involving products of combustion (H$_2$O) and with $\Omega_r$ this due to radicals and intermediates (H, OH, H$_2$O$_2$, and HO$_2$). In the remaining of the paper we’ll refer to $(D_{th}/Le_{H_2}) \nabla^2 \xi_H$ as the diffusion term (Term I) and to $\Omega_p + \Omega_r$ as the source term (Term II).

In order to quantify the occurrence of differential diffusion at the front of the combustion wave (either a diffusion-limited deflagration or a spontaneous ignition front), we employ a surface tracking technique as in Ref. [15]. An expression for the displacement speed of a iso-surface of scalar $i$ can be derived from Eq. (8) to obtain

$$S_d = -\frac{\dot{\omega}_i}{\rho |\nabla Y_i|} - \frac{\nabla \cdot (\rho D_i \nabla Y_i)}{\rho |\nabla Y_i|}$$

(11)

We evaluate Eq. (11) on the $Y_{H_2} = 8.5 \times 10^{-4}$ iso-contour, which corresponds approximately to the location of maximum heat release rate through most of the simulation. Also, we indicate with $\mathbf{n}$ the normal to the combustion front positive into the unburnt mixture. The normalized curvature of the front is $\kappa = \delta \mathbf{n} \cdot \mathbf{n}$. It is negative when the front is convex in the direction of the normal (i.e. towards the unburnt mixture). Additionally, in order to characterize the local heat release rate and displacement speed response to flame stretch we use the Karlovitz number (see Refs. [16,17]), defined as

$$Ka = Ka_T + Ka_C$$

(12)
Table 4: List of physical times at 1%, 5%, 20%, and 50% total heat release.

<table>
<thead>
<tr>
<th>Variable</th>
<th>% total heat release</th>
<th>Time (ms) B (15 K)</th>
<th>Time (ms) C (30 K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau_1$</td>
<td>1</td>
<td>1.480</td>
<td>1.0</td>
</tr>
<tr>
<td>$\tau_5$</td>
<td>5</td>
<td>1.914</td>
<td>1.3</td>
</tr>
<tr>
<td>$\tau_{20}$</td>
<td>20</td>
<td>2.296</td>
<td>1.6</td>
</tr>
<tr>
<td>$\tau_{50}$</td>
<td>50</td>
<td>2.601</td>
<td>2.0</td>
</tr>
</tbody>
</table>

where

$$K_a \equiv (nn : \nabla u + \nabla \cdot u)\tau_F$$

is the normalized tangential strain rate, with

$$nn : \nabla u = \sum_i \sum_j n_{ij} n_{ij} \partial u_i / \partial x_j,$$

and

$$K_a \equiv (S_d / S_L)\delta_F \nabla \cdot n = (S_d / S_L)\kappa$$

is the curvature component.

4 Results and discussion

Figures 1 and 2 show several instantaneous images of the contour plots during the ignition event for an initial temperature stratification of 15 and 30 K (cases B and C). The three columns represent heat release rate (normalized by the maximum heat release rate at each instant), $\xi_H$, and the sum of the diffusive and reactive sources for $\xi_H$ (see Eq. (10)). In each plot, the black solid lines represent isoscalar surfaces at $Y_{H_2} = 8.5 \times 10^{-4}$, which we take as the location of the flame front. The four snapshots from top to bottom were captured at approximately 1%, 5%, 20% and 50% total heat release. Table 4 summarizes the actual physical times for cases B and C. Because of the initial temperature distribution, isolated pockets of hot reactive mixture begin to ignite very early in the process. These igniting kernels lead to a localized depletion of hydrogen and production of water. Because of the differential diffusion of $H_2$ into the igniting kernel as opposed to the diffusion of water out of the chemically active region, there occurs a net accumulation of atomic H. In this early stage of the ignition process ($t \leq \tau_5$), the right hand side of Eq. (10) is positive, leading to an increase in $\xi_H$. Figures 3 and 4 show the profiles of several scalars across igniting kernels at $t = \tau_1$. The localized peaks in $\xi_H$ correlate to peaks in temperature and heat release rate. Under increased temperature stratification conditions, excess $\xi_H$ may lead to undesirable enhancement in NO$_x$ formation, even if higher equivalence ratios are required to reach a temperature of 1800 K and above necessary for the formation of NO$_x$. The magnitude of the diffusion and reaction source terms (indicated as Term I and Term II) is far greater for $T_{r.m.s.} = 30$ K than for $T_{r.m.s.} = 15$ K due to steeper temperature gradients, which result in smaller igniting kernels. The influence of vortical motions on differential diffusion in these early stages of the ignition event seems to be connected with the effect of vortices on the temperature field. As it has been observed in [9], the tangential component of stretch creates elongated regions of high temperature gradient (extensive straining) and low curvature alternating with regions of low gradient and high curvature (compressive straining). Similar arguments hold for $\xi_H$ contours. In these early moments of the ignition event, while the accumulated heat release is within 1% and 10% of the total, iso-surfaces of temperature, $Y_{H_2}$ and $\xi_H$ overlap for the most part, indicating that differential diffusion is controlled by localized fuel consumption. As ignition fronts appear ($t = \tau_{20}$), we observe that the shortage of atomic H is
Figure 1: Sequence of contours for case B ($T_{r.m.s.} = 15$ K) at 1%, 5% 20% and 50% total heat release from top to bottom (see Table 4 for actual times). The three columns show heat release rate (normalized), $\xi_H$ and the right hand side of the transport equation of $\xi_H$ (see Eq. (10)).
Figure 2: Sequence of contours for case C ($T_{r.m.s.} = 30$ K) at 1%, 5% 20% and 50% total heat release from top to bottom (see Table 4 for actual times). The three columns show heat release rate (normalized), $\xi_H$ and the right hand side of the transport equation of $\xi_H$ (see Eq. (10)).
Figure 3: Profiles of along a in Figure 1 (case B) at 1% of heat release.

Figure 4: Profiles along a in Figure 2 (case C) at 1% of heat release.

Figure 5: Profiles at a location of low curvature along b in Figure 1 (case B) at 20% of heat release. At the flame front, the displacement speed is \( S_d/S_L = 0.42 \).

Figure 6: Profiles at a location of negative curvature along c in Figure 1 (case B) at 20% of heat release. At the flame front, the displacement speed is \( S_d/S_L = 1.0 \).
concentrated in elongated structures aligned with the fronts in areas of low front curvature, while regions of high (negative) front curvature do not display such features. This characteristic is apparent both in case B and C. The profiles taken along segment lines shown in Figures 5 and 6 highlight how radically different is the balance of the diffusion and source terms for $\xi_H$ in a deflagration (Figure 5) and a spontaneous ignition front (Figure 6). Later in the ignition ($t = \tau_{50}$), a strong correlation between temperature and $\xi_H$ holds, both in the whole computational domain as well as along reacting fronts, as shown in Figures 7 and 8. For pockets of mixture with $\xi_H/\xi_0$ in excess of unity, the temperature reached at the end of the burn correlates very well with the equilibrium temperature of a hydrogen/air mixture of identical fuel to oxidizer mass ratio. Let us define $\xi_{H,max}$ as the maximum in the ensemble of $\xi_H$ values sampled from the computational domain. It is interesting to compare the value of $\xi_{H,max}$ during ignition of mixtures subject to different levels of temperature stratification ($T_{r.m.s.} = 3.75, 15,$ and $30$ K). Figure 9 shows that $\xi_{H,max}$ reaches a higher peak value as temperature stratification increases. Additionally differential diffusion occurs earlier and over a longer period of time for $T_{r.m.s.} = 30$ K as opposed to the lower level of stratification, $T_{r.m.s.} = 3.75$ K. This behavior correlates well with the heat release rate, shown in Fig. 10, even if the peak in $\xi_{H,max}$ is reached well before the peak in heat release rate. The global heat release rate is little affected by differential diffusion. It appears that differential diffusion slightly accelerates the occurrence of heat release and lowers the peak heat release rate by $\approx 5\%$ and $10\%$ for $T_{r.m.s.} = 15$ K and $T_{r.m.s.} = 30$ K respectively. As shown in [9], when temperature stratification increases, a growing part of the burn area production is due to deflagrations as opposed to spontaneous ignition fronts. Since differential diffusion is characterized by time scales which are comparable to deflagration time scales, one would expect that differential diffusion would affect deflagration fronts and not spontaneous ignition fronts. We distinguish among the effect of differential diffusion on macro quantities (such as global heat release rate and production of burnt area) and local flame dynamics. Figures 11 and 12 show the heat release rate along combustion
fronts with and without differential diffusion respectively. We observe that regions of high negative curvature are characterized by more intense burning, but this feature is absent from the case without differential diffusion, which displays a narrower distribution of heat release rate. This is a well known feature of lean premixed hydrogen flames (e.g. see Ref. [16]). However, in the present regime, highly curved regions are mostly associated with low temperature gradients and spontaneous ignition fronts where diffusive fluxes do not play a role. Hence, it is somewhat unexpected to find that differential diffusion affects heat release rate in highly curved segments of the combustion front. Figure 13 shows the distribution of heat release rate along deflagration fronts during peak heat release rate. Differential diffusion decreases the mean heat release rate, while it enhances its variance and its peak value. This is coherent with the findings on the role played by differential diffusion smoothing the global heat release (see Fig. 10). However, Figure 14 shows that differential diffusion hardly affects the fraction of burn area generated by deflagrations. Figures 13 and 14 seem to be in disagreement as differential diffusion has strong and negligible effect respectively. However, one has to bear in mind that burn area production and total heat release rate are integral quantities, which tend to diminish the effects of localized peaks in heat release rate. We conclude that differential diffusion hardly impacts macro combustion quantities. Further statistical data is presented in Figure 15, where the displacement speed is plotted against the total Karlovitz number at the combustion front. At these conditions, curvature induced stretch (\(K_{aC}\)) greatly dominates over tangential stretch (\(K_{aT}\)) as a whole. This is coherent with the high displacement speeds due to spontaneous igniting fronts at locations of high curvature. One notices that the samples from a deflagration fall in the region of low \(K_a\) and a large degree of scatter is present in the data, as reported previously for lean premixed hydrogen/air flames subject to turbulence [16]. However, along deflagration fronts, the balance among tangential strain and curvature induced stretch is less biased and we recognize the effects of differential diffusion and the diffusive-thermal instability characteristic of lean hydrogen flames, which has been reported in the DNS of Im et al. [16].
Figure 11: Heat release rate versus normalized curvature $\kappa$ at $t = \tau_{50}$ for a simulation with differential diffusion (case C).

Figure 12: Heat release rate versus normalized curvature $\kappa$ at $t = \tau_{50}$ for a equal diffusivity ($Le = 1$) run (case E).

Figure 13: Distribution of heat release rate along the deflagration fronts ($S_d/S_L < 1.1$) at $t = \tau_{50}$ for $T_{r.m.s.} = 30$ K for case with and without treatment of differential diffusion.

Figure 14: Fraction of burn area production associated with a deflagration ($S_d/S_L < 1.1$) for different levels of initial stratification and unit Lewis number formulation.
5 Conclusions

The occurrence of differential diffusion during the ignition of a temperature stratified lean hydrogen/air mixture at HCCI-like conditions was studied for different levels of stratification. It was found that differential diffusion effects are most prominent for the case of large temperature stratification. Differential diffusion affects the local characteristics of combustion in two ways. It creates pockets of peak temperature and heat release rate in regions of excess atomic H mass fraction during the early phase of the ignition. This is due to hydrogen rushing into igniting kernels faster than products (water) leaving. Eventually, kernels in excess of $\xi_H$ reach higher temperatures, which are well explained using equilibrium temperature arguments. Later in the simulation, differential diffusion enhances heat release rate in regions of high negative curvature along deflagration fronts. This finding is consistent with previous work [16] on lean hydrogen/air premixed flames, but it is somewhat unexpected in the present regime in which highly curved regions promote spontaneous ignition fronts rather than deflagrations in diffusive-reactive balance.

Despite evident local effects, for the level of differential diffusion observed and the limited role played by deflagrations (as opposed to spontaneous ignition fronts), macro combustion characteristics such as total burn time, and heat release rate are only slightly affected by differential diffusion, which decreases the peak heat release rate merely by $\approx 10\%$ in the case of the highest temperature stratification ($T_{r.m.s.} = 30$ K). Overall, burn rates are left unaffected. It can be expected that under higher temperature stratification, deflagrations are promoted to a greater extent, and overall heat release rate would be affected more, thus posing a modeling challenge. Additionally, the existence of pockets of high temperature products at ignition kernels, which persist for extended period of time, might result in the production of NO$_x$. The investigation of the role of differential diffusion in the generation of NO$_x$ will be the subject of further studies.

References


