A Numerical Study of Laminar Flames Propagating in Stratified Mixtures

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Abstract: Numerical simulations are carried out to study flame propagation in laminar stratified fuel-air mixtures. Studies are carried out in hydrogen-air and methane-air mixtures. A 30-species 184-step skeletal mechanism is employed for methane oxidation and a 9-species 21-step mechanism for hydrogen oxidation. The study seeks to provide an improved understanding of possible differences in the local flame speed at an equivalence ratio in the compositionally stratified mixture from the speed in a homogeneous mixture at the same equivalence ratio. Flame speed and temperature profiles are evaluated and compared with corresponding values for homogeneous mixtures. As shown in prior experimental work, the numerical results suggest that when the flame propagates from a richer mixture to a leaner mixture, the flame speed is faster than the corresponding speed of the homogeneous mixture. The flame zone thickness is observed to be thinner in the stratified mixture resulting in sharper gradients. As a result, the rate of diffusion of heat and species increases resulting in increased flame speed. The effects become more pronounced in leaner mixtures. The stratification gradient influences the results with shallower gradients showing less difference in flame speeds between stratified and homogeneous mixtures. The comparative effect of thermal diffusion and species diffusion on the differences in flame speed is studied. It is shown that the species diffusion effect is more important.

Keywords: stratified-charge combustion, stratified hydrogen/air mixture, stratified methane/air mixture, compositional stratification, flame speed

1. Introduction

Flame propagation in compositionally stratified mixtures occurs in many applications including internal combustion engines with direct fuel injection and fires induced by leakage of fuel from storage tanks. Modeling these flames is important in improving the understanding of the physics of flame propagation and the design of the devices. For example, flame propagation speed in the combustion chamber of an internal combustion engine is one of the factors that determine the efficiency of the engine. Compositional stratification is employed in low temperature combustion engines to extend the high and low load operating limits of the engines [1-6]. Stratification also exists in direct-injection spark-ignited hydrogen and natural gas fueled engines. In these engines, direct injection is employed to extend the lean limit of operation of the engines [7-9]. Prior work suggests that flame speeds in stratified mixtures are greater than in homogeneous mixtures at the corresponding equivalence ratios. If this is the case, computational models that approximate the local flame speed at an equivalence ratio to be the flame speed in a homogeneous mixture with the same equivalence ratio would not be suitable for optimizing such engines. It is important to understand how the speed depends on the stratification. This motivates the current work.

The focus of this work is on flame propagation parallel to the compositional gradient. Kang and Kyritsis [10-12] measured flame speeds in stratified methane-air mixtures using high-speed optical visualization to

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observe the flame positions. A relatively rich mixture of known composition was diffused into the combustion chamber from the top of the chamber. This diffusion was opposed by a very mild counter-flow of air from the bottom of the chamber. The compositional stratification was thus achieved by the convective-diffusive balance in the chamber. The results showed that the flame propagated from the richer to leaner mixture with a faster speed than the laminar flame speed in a homogeneous mixture corresponding to the local equivalence ratio. A significant extension of the lean flammability limit was observed and explained by “back-supported” effect due to the heat diffusion from the burned gases where the temperature is higher into the leaner mixture. A similar method has been adopted to explore the propagation behavior of laminar flames into gradually richer methane/air mixture [13]. The flames are ignited in locations with close-to-stoichiometric composition. Note that the flame speed is a maximum at this composition and it decreases as equivalence ratio increases. As the flame propagates into the richer mixture, the flame is “back-supported” by heat diffusion from the region with higher flame temperature. This leads to flame speeds that are higher than the ones in homogeneous mixtures corresponding to the local equivalence ratio in the stratified mixture. Kitagawa et al. [14] investigated the flame propagation in a stratified hydrogen/air mixture. It was found that the lean flammability limit was extended by the stratification.

In addition to the experimental works cited above, Da Cruz et al. [15] have carried out numerical studies of freely propagating laminar methane/air flames in compositionally stratified mixtures. The initial configuration was that of fuel/air mixtures of different fuel concentrations with a diffusion interface at the center of the domain. The diffusion layer thickness between the two mixtures was initially a step function but grew in thickness as a result of diffusion. Results showed that the laminar flame speed was strongly affected by the equivalence ratio gradient. A change in the rate of diffusive transport of radicals and heat to the reaction zone was suggested as the key factor in explaining the behavior. All the studies cited above appear to agree on this explanation. In the current work, the compositional gradients considered are shallower than in the work of Da Cruz et al. [15] and are more representative of such gradients in engines [4]. Furthermore, the effect of Lewis number on the flame speed enhancement is studied. Lewis number is likely to be an important consideration because the explanation for the speed enhancement is based on changes in diffusive transport of heat and species.

The objective of this work is to employ direct simulations of the laminar flame propagation to understand the physics of how flame speed is related to the compositional stratification. The outline of the rest of the paper is as follows. In the next section, the numerical method and chemical kinetics mechanisms employed in this work are described. Results and discussion follow. The predicted flame speeds in stratified mixtures are compared with those in corresponding homogeneous mixtures. The comparative influence of thermal and species diffusion on “back-support” is evaluated. The paper closes with summary and conclusions.

2. Computational setup and chemical kinetics

The computations are carried out with the FLEDS (Flow Large-Eddy and Direct-Simulation) code. The code solves the compressible form of the Navier-Stokes equations for multicomponent gaseous mixtures with chemical reactions. The sixth-order compact finite-difference scheme of Lele [16] is employed to spatially discretize the governing equations. The resulting discretized equations are solved using the tridiagonal matrix algorithm. A fourth order Runge–Kutta scheme is employed to perform the time-integration. Boundary conditions are implemented using the Navier–Stokes characteristic boundary conditions method of Poinsot and Lele [17], which is extended to account for multicomponent transport by Anders et al. [18]. Chemical kinetic source terms are computed through an interface with CHEMKIN-like subroutines. The effective binary diffusion coefficient model for computing species diffusion, using the method of Bird et al. [19], is implemented. The code is written in FORTRAN 90 and parallelized using the message passing interface library. The code has been employed in prior studies for direct simulations of
laminar flames, turbulent flames, and large-eddy simulations of jets [20-22, 23].

The physical configuration studied in this work is that of an adiabatic flame propagating in a one-dimensional domain. The domain is divided into two parts as shown in Fig. 1. The left part contains the compositionally stratified unburned mixture. The right part contains a homogeneous fuel/air mixture. Part of the homogeneous mixture (the part to the right of the “initial flame position”) is initialized with the equilibrium temperature and composition of a burned equilibrium mixture. A linearly stratified gradient is specified in the left part. The initial species and temperature profiles in the flame are specified as follows:

\[
f(y) = \left(\frac{f_U + f_B}{2}\right) + \left(\frac{f_B - f_U}{2}\right) \tanh \left(\frac{y - y_c}{\delta}\right),
\]

where \(f(y)\) is a general parameter which can represent mass fraction of species \(Y_i\) or temperature \(T\) as a function of \(y\) location. \(y_c\) represents the location where \(f(y)\) is half-way between the maximum and minimum values. The parameter \(\delta\) is a measure of the flame thickness. \(f_B\) and \(f_U\) are the burned and unburned mixture values. The hyperbolic tangent profile has been selected in many prior numerical studies of mixing layers or to mimic the profile across a flame [24-32]. After the start of the calculation, a time period is required for the flame speed to equilibrate to that of the laminar flame corresponding to the homogeneous mixture. The distance from the initial flame position to the stratified mixture is selected such that the flame can stabilize and reach its steady speed and structure before propagating into the stratified region. The pressure is 1 bar. Periodic boundary conditions are imposed on boundaries parallel to the flame propagating direction.

The resolution of the domain is dependent on the flame thickness. The flame thickness in this study varies from 0.4 mm for the hydrogen flame at 300 K, 1 bar, and equivalence ratio of 1.0 to 0.6 mm for the methane flame under the same conditions. The flame is thicker for lower equivalence ratios. The grid points are uniformly distributed in the domain. The effect of grid resolution on the results was assessed. Prior studies of premixed laminar flame propagation by Wang and Abraham [32] showed that 10 cells in the diffusion layer are enough to resolve the flame speed and structure when using FLEDS. In this work, up to 20 cells are employed in the flame. Figure 2 shows results of temperature, heat release rate, H mass fraction, and OH mass fraction in a premixed flame for a mixture with \(\phi = 0.9\) when the grid resolution is progressively increased. It can be seen that the results with the 20 and 10 µm resolutions are about the same suggesting that 20 µm is adequate to resolve the flame. Notice that the flame thickness here is about 400 µm. The 20µm grid size corresponds to the resolution level that there are 20 cells employed in the flame. While not shown, the flame speeds with these two finer resolutions was determined to be 1.95 m/s in both cases. The flame speeds are over-predicted when using 40 µm and 100 µm resolutions. The study was repeated for a mixture with \(\phi = 0.6\) and the results are shown in Fig. 3. Once again, the results show that the grid independence is achieved with a resolution of 20 µm. These results are consistent with the earlier findings of Wang and Abraham [32].
Fig. 2. Temperature, heat release rate, and H, OH mass fraction profiles in homogeneous mixture when $\phi=0.9$ with four mesh resolutions.
The fuels employed in this study are hydrogen and methane. A 30-species 184-step skeletal mechanism [33] is employed for methane oxidation and a 9-species 21-step mechanism [34] for hydrogen oxidation. The flame speed predicted with the 30-species 184-step methane mechanism was compared with predictions from the GRI-Mech 3.0 mechanism. Fig. 4 compares the computed flame speeds at a pressure of 1 bar and unburned mixture temperature of 300 K. It can be seen that the 30 species skeletal mechanism shows agreement with the GRI-Mech 3.0 within about 3% for the range of equivalence ratios considered. The 9-species 21-step hydrogen mechanisms has been discussed and evaluated in the work of Owston [35]. Owston [35] compared heat release rates, flame speeds, peak temperatures, and species distributions with those calculated using a more detailed 30-step mechanism [36] and showed that results agree well between the two mechanisms. The differences between the flame speeds computed using the two mechanisms are within 5%.

Fig. 4. Computed and measured CH₄/air flame speeds for unburned temperature of 300 K at pressure of 1 bar using two mechanisms.
3. Results and discussion

Five cases of flame propagation in compositionally stratified mixtures are considered. Table 1 lists the conditions employed for the computations. In Cases 1, 2, 4 and 5, hydrogen is employed as fuel. Unity Lewis number assumption is adopted in Case 2. Case 2 provides a good contrast with Case 1 to show the effect of differential species diffusion and differences in thermal and species diffusion on flame propagation behavior in stratified mixtures. Case 3 uses CH$_4$ as fuel but has the same gradient of equivalence ratio ($\phi$) as the first two cases. The equivalence ratio distribution in the unburned stratified mixtures of first 3 cases varies linearly from 1 (stoichiometric) to 0 (no fuel) in 10 mm length along the flame propagation direction. This level of stratification comes from the measurement by Hwang et al. [4]. They studied the fuel distribution with fuel PLIF imaging in an optically accessible LTC engine. Early-injection is employed to create the fuel stratification and other conditions are also representative for stratified charge engines. The stratification gradient employed here is estimated from their equivalence-ratio maps. In Case 4, a lower gradient of stratification is employed. The equivalence ratio varies from 1 to 0.5 in 10 mm in the unburned mixture. The propagation behavior of flame in gradually richer mixture is studied in Case 5. The equivalence ratio changes linearly from 0.5 to 1.5 in 10 mm in the unburned mixture. The unburned mixture temperature and pressure are kept the same for all cases at 300 K and 1 bar, respectively.

Separate simulations are carried out to determine the steady laminar flame speeds and flame profiles in homogeneous mixtures at different equivalence ratios ($\phi = 1.4, 1.3, 1.2, 1.1, 1, 0.9, 0.8, 0.7, 0.6, 0.5$). The conditions for these simulations are listed in Table 2. Each group of cases relates to the corresponding stratified mixture case by sharing the same kind of fuel, unburned mixture temperature, pressure and Lewis number assumption. The data from homogeneous mixture cases are used to compare with the results from stratified cases at corresponding equivalence ratio and unburned mixture temperature.

### Table 1
Summary of simulation cases for stratified mixture

<table>
<thead>
<tr>
<th>Case ID</th>
<th>Fuel</th>
<th>Lewis number</th>
<th>$T_U$</th>
<th>Pressure</th>
<th>$\phi$ distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>H$_2$</td>
<td>Non-unity</td>
<td>300 K</td>
<td>1 bar</td>
<td>$\phi=1$ to $\phi=0$</td>
</tr>
<tr>
<td>2</td>
<td>H$_2$</td>
<td>Unity</td>
<td>300 K</td>
<td>1 bar</td>
<td>$\phi=1$ to $\phi=0$</td>
</tr>
<tr>
<td>3</td>
<td>CH$_4$</td>
<td>Non-unity</td>
<td>300 K</td>
<td>1 bar</td>
<td>$\phi=1$ to $\phi=0$</td>
</tr>
<tr>
<td>4</td>
<td>H$_2$</td>
<td>Non-unity</td>
<td>300 K</td>
<td>1 bar</td>
<td>$\phi=1$ to $\phi=0.5$</td>
</tr>
<tr>
<td>5</td>
<td>H$_2$</td>
<td>Non-unity</td>
<td>300 K</td>
<td>1 bar</td>
<td>$\phi=0.5$ to $\phi=1.5$</td>
</tr>
</tbody>
</table>

### Table 2
Summary of simulation cases for homogeneous mixtures

<table>
<thead>
<tr>
<th>Group ID</th>
<th>Fuel</th>
<th>Lewis number</th>
<th>$T_U$</th>
<th>Pressure</th>
<th>$\phi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>H$_2$</td>
<td>Non-unity</td>
<td>300 K</td>
<td>1 bar</td>
<td>0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1, 1.1, 1.2, 1.3, 1.4, 1.5</td>
</tr>
<tr>
<td>2</td>
<td>H$_2$</td>
<td>Unity</td>
<td>300 K</td>
<td>1 bar</td>
<td>0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1</td>
</tr>
<tr>
<td>3</td>
<td>CH$_4$</td>
<td>Non-unity</td>
<td>300 K</td>
<td>1 bar</td>
<td>0.5, 0.6, 0.7, 0.8, 0.9, 1</td>
</tr>
</tbody>
</table>

3.1 Laminar flame speeds for stratified and homogeneous hydrogen/air mixtures

Local laminar flame speeds at selected equivalence ratios from the stratified mixture are compared with those in homogeneous mixtures at the same equivalence ratio. The flame speed is calculated by evaluating the movement of flame position. Two methods are adopted to define the flame position during propagation. The first method uses the position of the peak of heat release rate as the current flame position. The second method employs the position where the unburned gas temperature rises by 50 K. The flame position defined
by the method 1 is indicative of the position of the reaction zone in the flame. Method 2 is more indicative of the leading edge of the flame. The distance between two flame positions predicted by the two methods is dependent on the flame thickness. For transient flame propagation through a stratified mixture, this distance varies as the flame thickness changes during propagation. This, in turn, influences the estimated flame speed. For steady flame propagation in homogeneous mixtures, the calculated flame speeds are not influenced by the characterization of flame position as the flame profile does not change.

A comparison between the laminar flame speeds of the homogeneous calculations (Group 1 in Table 2) and the laminar flame speed as a function of the local equivalence ratio for Case 1 in Table 1 is shown in Fig. 5. Flame speeds estimated by the two methods are plotted in the figure. The local equivalence ratio is defined as the average between two flame positions based on method 1 or method 2.

![Graph](image)

**Fig. 5.** Comparison of local flame speed in a stratified hydrogen/air mixture with the flame speed in a homogeneous mixture at the corresponding equivalence ratio (Le ≠ 1).

The results indicate that flame propagates faster in the stratified mixture than in a corresponding homogeneous mixture with the local equivalence ratio of the stratified mixture. This is consistent with the finding reported in Refs. [10-12,15]. This can be related to the mass and thermal diffusion rates from the burned region which are different in stratified and homogeneous mixtures. The unburned temperature and radical concentrations on the richer side of the flame in the stratified mixture are higher compared to the corresponding homogeneous mixture. This “back-supports” the transient flame as it propagates into leaner regions in the stratified mixture. In order to better understand the mechanisms responsible for the difference in speeds, the temperature, H and OH mass fractions, and heat release rates for the homogeneous and stratified mixtures are shown in Fig. 6. In the stratified case, the profiles are taken when the equivalence ratio at the flame position defined by method 1 is 0.5. The flame positions of the two cases are shifted to the same point for comparison.
Higher burned gas temperature and greater concentration of radicals in the burned gas are noticeable in the stratified mixture. The higher temperature reflects the higher equivalence ratio in the burned mixture behind the flame when the mixture is stratified. This higher temperature results in greater diffusion rate of heat into the unburned mixture which, in turn, contributes to greater fuel decomposition and higher reaction rates compared to the homogeneous mixture. The concentrations of radical species involving H and OH are also higher in the upstream “richer” burned mixtures. These radical species diffuse into the flame region and contribute to an increase in heat release rate. The net effect of the increased diffusion rates of heat and species is an increase in flame speed. These effects become more prominent in leaner mixture. The stratified flame speed (calculated by method 2) at $\phi = 0.9$ is 5% higher than the corresponding homogeneous flame speed, while the difference increases to 70% when $\phi = 0.4$. This may also be influenced by the increase in the chemical time scale in leaner mixtures. When the flame reaches the leaner mixture, it slows down, and allows more heat and radical molecules to diffuse into flame region from the richer burned side. As a result, the “back-supporting” effect becomes more dominant. Counteracting this will be slower diffusive transport on account of lower temperatures.

It is also interesting to consider the differences in the flame speeds derived by the two methods. The figure clearly shows that the flame edge/tip travels faster than the reaction zone. This may be related to the transient thickening of the flame as it propagates into the leaner mixture. It is also worth mentioning that the flame positions were observed by high-speed photography in the experimental work by Kang and Kyritsis.
[10-12]. The definition of flame position by its optical properties is likely different from that obtained by either of the methods adopted here. So the measured flame speeds and the corresponding conclusions may be different from the predicted results.

3.2 Laminar flame speeds for hydrogen/air mixtures with unity Le number assumption

From a modeling perspective, it is interesting to assess the effect of the unity Le number assumption on the predicted results. The unity Le assumption is sometimes employed in modeling the flames. Consider Case 2 of Table 1 which is identical to Case 1 with the exception that Le =1 in Case 2. The corresponding homogeneous results are obtained from the simulations from Group 2 of Table 2. As before, the predicted flame speeds for the stratified case at various local equivalence ratios are compared with the flame speeds in homogeneous mixtures at the same equivalence ratio. The comparison is shown in Fig. 7. The temperature, heat release rates, and H and OH mass fractions, for the homogeneous and stratified mixtures are shown in Fig. 8. Note that the corresponding results for the non-unity Le case were presented in Figs. 5 and 6, respectively. Recall that ‘method 1’ and ‘method 2’ denote two ways in which the flame speeds are determined in the stratified-charge simulations. The Le = 1 assumption reduces the molecular diffusivity of molecules like H$_2$, H and OH when compared to the results presented earlier with non-unity Le number. As a result, their concentrations in the flame are not noticeably different from that of the flame in the homogeneous mixture unlike in the earlier case where Le ≠ 1 (compare results of Figs. 6 and 8). The net effect is that the heat release rates are also not very different and the flame speeds for the stratified and homogeneous mixtures are not noticeably different by “method 1” and only different by less than 5% by “method 2” (compare results of Figs. 5 and 7).

These results suggest that computations with the Le =1 assumption may not capture the higher flame speeds of stratified mixtures. It is interesting to note that the primary difference between Cases 1 and 2 lies in the molecular diffusivity of the species. The reduced diffusivity of light species such as H$_2$ and H weakens the “back-supporting” effect caused by higher concentration of radicals in the richer burned region. The thermal stratification behind the flame still exists as the burned products from the richer mixture are at higher flame temperature. This argument appears to suggest that the increased rate of diffusive transport of excess radical concentrations in the burned region is more controlling than that of heat in “back-supporting” stratified flame propagation.
Fig. 7. Comparison of local flame speed in a stratified hydrogen/air mixture with the flame speed in a homogeneous mixture at the corresponding equivalence ratio (Le = 1).
3.3 Laminar flame speeds for methane/air stratified mixture

It is interesting to assess the impact of changing the fuel on the results. In this section, results will be presented for methane, often considered as a surrogate for natural gas. Methane flame speeds are lower than those of hydrogen and flame is thicker. The stratified case is identified as Case 3 in Table 1 and the corresponding homogeneous simulations are those of Group 3 in Table 2. Figure 9 shows the comparison of predicted flame speeds in the stratified mixture, with the two methods, and in the homogeneous mixture. Interestingly, the flame speed based on the location of the peak heat release rate (method 1) does not show a significant difference from the flame speed in the corresponding homogeneous mixture. This result is consistent with the result in Fig. 7 where the flame speed in the stratified hydrogen/air mixture did not differ from the flame speed in the corresponding homogeneous mixture when the $Le = 1$ assumption is made. On the other hand, the flame speed based on the location of the flame edge shows a significant difference with the flame speed higher in the stratified mixture, by as much as 50%. This may reflect the effect of the higher thickness of the methane flame relative to the H$_2$ flame. In the H$_2$ flame, the equivalence ratio gradient across the flame is small. In the case of the thicker methane flame, the equivalence ratio at the leading edge of the flame is lower than that in the region where the maximum heat release rate occurs. Note that the methane flame gets thicker as it propagates into the leaner mixture. This implies that the leading edge moves faster and this may explain the difference.
Fig. 9. Comparison of local flame speed in a stratified methane/air mixture with the flame speed in a homogeneous mixture at the corresponding equivalence ratio (Le ≠ 1).

3.4 Laminar flame speeds for hydrogen/air mixtures with different stratification gradient

As shown above, flame propagation is affected by the compositional stratification. Greater diffusion of heat and species from the burned region is believed to “back-support” the flame when it is propagating into leaner mixtures. It can be expected that the gradient of stratification has an effect on this behavior. In Case 4, the unburned mixture has a compositional gradient that is half the value of the gradient in Case 1. In the unburned mixture of Case 4, the equivalence ratio varies linearly from 1 to 0.5 in 10 mm, while the value changes from 1 to 0 in the same distance in Case 1.

Figure 10 shows the flame speeds evaluated by method 1 and method 2 in the compositionally stratified mixture and the flame speeds in the homogeneous mixture at corresponding equivalence ratio. In general, the flame speeds in the stratified mixture are higher than the corresponding flame speeds in the homogeneous mixture, but the differences are less than in Case 1 shown in Fig. 5. The temperature, heat release rates, and the H and OH mass fractions are compared with the results of Case 1 and the homogeneous mixture when \( \phi = 0.6 \) in Fig. 11. The results of Case 4 lie between the results of Case 1 and those of the homogeneous mixtures. Due to the lower gradient of compositional stratification, the thermal diffusion and mass diffusion from the burned side to the flame are reduced. This results in lower burned temperature, heat release rates and mass fractions of the radical species. A comparison of the results of Cases 1 and 4 shows that the “back-supporting” effect is influenced by the compositional gradient. When the flame propagates from a stoichiometric to leaner mixture, lower compositional gradient less “back-supporting” effect and the differences between the results in the stratified and corresponding homogeneous mixtures are lower, as expected.
Fig. 10. Comparison of local flame speed in a stratified hydrogen/air mixture (Case 4) with the flame speed in a homogeneous mixture at the corresponding equivalence ratio.
Fig. 11. Temperature, heat release rate, H, OH mass fraction profiles in a stratified mixture at the local equivalence ratio of $\phi = 0.6$ for Cases 1 and 4 compared with the profiles in a homogeneous mixture at $\phi = 0.6$.

3.5 Laminar flame speeds in hydrogen/air mixtures with increasing equivalence ratio

The propagation behavior of flames through gradually richer unburned mixture is studied in Case 5. The equivalence ratio varies linearly from 0.5 to 1.5 in 10 mm. This composition gradient has the opposite value of the gradient in Case 1. For laminar flames in homogeneous hydrogen/air mixture, the peak flame speed occurs when the equivalence ratio $\phi \approx 1.6$. Thus the flame speed is expected to increase during the propagation in Case 5. The results of flame speeds in the stratified mixture are compared with the flame speeds in homogeneous mixtures at corresponding equivalence ratio in Fig. 12. Temperature, heat release rate, mass fractions of H and OH are plotted in Fig. 13 at a local equivalence ratio of 0.8 along with the results of Case 1 and homogeneous mixtures for $\phi = 0.8$. Compared with the gradually leaner stratification in Case 1, the gradually richer stratification does not have a noticeable effect on the propagation behavior of hydrogen/air flame. The mass fractions of radicals such as H and OH in the stratified mixture in Case 5 are very similar to those in the homogeneous mixtures, indicating that the molecular diffusion does not show much difference.

The difference between the propagation speeds of flames propagating into gradually leaner and gradually richer compositional gradients can be explained as follows. When the flame is propagating into a gradually leaner mixture, the upstream richer composition creates more radicals than the leaner mixture would generate if the mixture were homogeneous. The radicals diffuse into the unburned mixture and increases the reaction rate and flame speed. In gradually richer mixture, the concentration of radicals can be assumed to be greater in the richer mixture into which the flame propagates compared to the leaner mixture from which the flame propagates. It would appear that the diffusion of the radicals from the richer mixture to the leaner mixture should reduce the flame speed. But, it does not because the radicals in the richer mixture are generated only after combustion initiates there and at this stage the effect of the stratification is not important any longer. As a result, the molecular diffusion does not affect the flame propagation speed significantly. In fact, the same argument would hold for thermal diffusion although, as pointed out earlier, the transport of heat appears to play a secondary role in modifying the flame speed compared to the transport of radicals.
Fig. 12. Comparison of local flame speed in a stratified hydrogen/air mixture (Case 5) with the flame speed in a homogeneous mixture at the corresponding equivalence ratio.
Fig. 13. Temperature, heat release rate, H, OH mass fraction profiles in gradually leaner (Case 1) and gradually richer (Case 5) stratified mixtures at local $\phi = 0.8$ and homogeneous mixture at $\phi = 0.8$.

4. **Summary and conclusions**

The propagation of hydrogen/air and methane/air laminar flames at atmospheric pressure in compositionally stratified mixtures is numerically studied. Consistent with prior findings reported in the literature, the local flame speed is higher in the compositionally stratified mixture compared to that in the homogeneous mixture at the same equivalence ratio. Detailed analysis of results confirms that this effect is due to the transport of heat and radicals from the richer burned mixture behind the flame to the leaner mixture in the flame. This effect is referred to as the “back-support” effect. The effect is more pronounced in hydrogen/air mixtures than methane/air mixtures because of increased diffusion effects. In fact, it is shown that the species diffusion effects are more important than thermal diffusion effects in determining the contribution to “back-support” in hydrogen/air flames. The “back-support” effect is also influenced by the compositional gradient. It is reduced when the compositional gradient decreases. Flame propagation into gradually richer stratified hydrogen/air mixture is also studied. In this case, there is negligible influence of the stratification gradient.

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Reference


