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Mitigation of preferential diffusion effects by intensive strain in lean premixed hydrogen flamelets

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ABSTRACT

The interplay between strain and preferential diffusion in lean premixed hydrogen flamelets is investigated numerically. Lean conditions are established at an equivalence ratio of 0.5. Detailed chemistry, one-dimensional simulations are performed on a reactants-to-products counterflow configuration, both including and artificially excluding preferential diffusion effects. A comprehensive analysis of the flame physical properties is performed, showing that preferential diffusion tends to weaken the flame as compared to the case where it is artificially suppressed, as it triggers a local leaning of the mixture ahead of the flame front. Counterintuitively, strain is observed to counteract or limit this preferential diffusion effect, with the peaks of radicals and reaction rate, flame thickness, and consumption speed, progressively approaching and in some cases overtaking the corresponding solution obtained with equal diffusivities as strain increases. This is shown to be a consequence of the fluid elements being increasingly preferentially transported in the flame tangential direction rather than diffusing in the flame normal direction. Hence, the flame weakening effect due to different diffusive fluxes of fuel and oxidizer across the flame front is progressively compensated by their differential transport on the flame tangential direction triggered by increasing applied strain rate, which instead enables an overall enrichment of the burning mixture. This analysis provides a different view as compared to previous studies attributing to strain an enhancing influence on the effects of preferential diffusion. In this work the opposite interpretation is proposed instead, where strain acts as a limiting factor to the weakening effect of preferential diffusion on lean hydrogen flames.

1. Introduction

Recent progress in the power and transportation sectors have identified hydrogen as one of the most promising candidates to tackle the yearly increasing energy demand and the climate emergency. In the last decades, research efforts have focused on the possibility to burn hydrogen in lean premixed conditions, where the lower adiabatic flame temperature allows to decrease NO_x formation via the thermal route. In fact, hydrogen can sustain leaner burning regimes than typical hydrocarbon-based fuels thanks to its high reactivity and lower heating value [1,2]. However, flashback and uncontrolled flame propagation that are typical of this regime are amplified in presence of hydrogen due to its very high flame speed [3], its ability to auto-ignite [4], and its very high diffusivity [5].

Many recent studies have tried to shed light on the effects of preferential and differential diffusion in hydrogen lean premixed flames. It is worth noting that for preferential diffusion effects it is generally intended those associated to hydrogen's higher molecular diffusivity with respect to the other species [6], which is technically different than differential diffusion effects (sometimes referred to also as Lewis number effects), which are related to hydrogen's different molecular diffusivity with respect to its thermal diffusivity. However, this distinction is not yet uniquely defined in literature, and the terms are often used interchangeably. In the remainder of this paper we will refer to preferential diffusion due to the effects associated to mixture fraction variation, to be discussed later. In a one-dimensional, planar, lean premixed unstretched hydrogen flame (flamelet), the mixture fraction was observed to exhibit a local dip in the proximity of the flame [7], which can be interpreted as a local leaning of the burning regime because of different diffusion velocities between fuel and oxidizer caused by their non-equal diffusivity characteristics. Two-dimensional thermodiffusive instabilities also play a major role in hydrogen lean premixed flames. Following the growth rate relation of the perturbation derived by Bradley et al. [8], for cases with effective Lewis number below unity such as lean hydrogen-air mixtures, the propagation of these instabilities is intrinsically unstable, and thus self-amplifying.

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These instabilities have been observed to be affected by the equivalence ratio, preheat temperature, and pressure [9]. Another interesting property is the behaviour of lean hydrogen flames under stretched conditions. Unlike hydrocarbon fuels, in fact, the consumption speed of the lean hydrogen flame has been shown to increase with stretch in both numerical [10] and experimental studies [11] of curved laminar spherical flames, enabling a negative Markstein length. This feature has been identified as the responsible for the self-amplifying propagation of thermodiffusive cells: a locally positively (negatively) curved flame front will experience a further increase (decrease) in consumption speed that will further curve the flame front and thus amplify the instability propagation [12]. In light of this, together with the flame area increase, stretch has been identified as the main responsible for the increase of consumption speed of a thermodiffusive-unstable flame with respect to the unstretched hydrogen flame [9]. Turbulence has been recently shown to further enhance this increase in consumption speed due to the turbulence-enhanced curvature fluctuations, and to lead to super-adiabatic flame temperatures [13].

While the strong interaction between the curvature part of stretch and preferential diffusion has been extensively investigated in past studies, very few studies exist on flame tangential strain rate, i.e. the other contributor to stretch. Due to hydrogen's negative Markstein length, the consumption speed in hydrogen flames shows an increasing trend with increasing strain rate [14], just like in positively curved flame fronts. Furthermore, hydrogen can sustain very high strain rates [2], and the peak heat release rate has been shown to increase with strain [15]. Similar trends are observed for the flame temperature [3], while the opposite has been recently highlighted for NO_x emissions [16]. Strain has been also indicated as responsible for delayed lean blow-off in bluff body stabilized laminar flames [17]. However, the interaction of these distinctive hydrogen burning characteristics under strained conditions with hydrogen preferential diffusion is still unclear.

The purpose of the present study is to shed light on the way strain influences the preferential diffusion behaviour in lean premixed hydrogen flames. Results show that, in contrast to previous studies where strain is generically identified as a contributor to thermodiffusive instabilities [13] and preferential diffusion effects [17], strain rate mitigates the importance of cross-flame diffusion, ultimately limiting the impact of preferential diffusion on the flame global burning properties.

2. Setup and governing equations

Detailed chemistry one-dimensional analyses are performed for pure-hydrogen, lean premixed, strained laminar flamelets in a reactants-to-products counter-flow configuration. The flame configuration is sketched in Fig. 1 and was previously found to be the most suitable for this type of analysis involving high strain rates [16]. Simulations are run with the one-dimensional solver CHEM1D [18] for a range of applied strain rates from $a = 100\ \mathrm{s}^{-1}$ to $a = 10000\ \mathrm{s}^{-1}$. The reader is also invited to read Section 5 in the supplementary material to compare these strain regimes to practical turbulent flows. Detailed kinetic data of reactions from Conaire mechanism [19] are used, along with a multi-component diffusion model [20] including Soret and Dufour effects and with transport properties computed using the EGLIB library [21]. The reactants temperature is fixed to 300 K so that the most favourable conditions for the observation of preferential diffusion effects are established [9]. For the investigated setup, the set of conservation equations solved is re-arranged as follows [22]:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_x)}{\partial x} = -\rho K \tag{1a}$$

$$\frac{\partial(\rho Y_k)}{\partial t} + \frac{\partial(\rho u_x Y_k)}{\partial x} = -\frac{\partial(\rho V_{x,k} Y_k)}{\partial x} + W_k \dot{\omega}_k - \rho K Y_k \tag{1b}$$

$$\frac{\partial \rho K}{\partial t} + \rho u_x \frac{\partial K}{\partial x} = \frac{\partial}{\partial x}\left(\mu \frac{\partial K}{\partial x}\right) + \rho_\mathrm{p} a^2 - \rho K^2 \tag{1c}$$

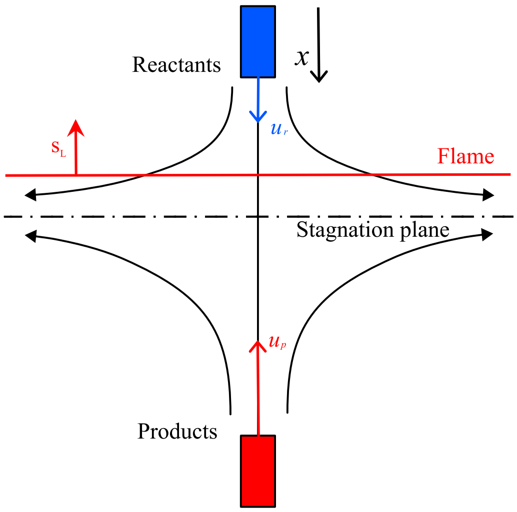

Fig. 1. Sketch of the reactants-to-products or fresh-to-burnt counter-flow premixed strained flame configuration.

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho u_x h}{\partial x} = \frac{\partial q}{\partial x} - \rho K h \tag{1d}$$

where ρ is the mixture density, u_x is the velocity across the longitudinal axis x of the flamelet, Y_k is the mass fraction of a generic species k, W_k is the molar mass of k, $\dot{\omega}_k$ the molar rate of production of k, $V_{x,k}$ is the diffusion velocity of k along x, ρ_p is the density of the injected products mixture, a is the applied strain rate, K is the local strain rate, h is the enthalpy and q is the total heat flux. Note that the unsteady term in the equations is reported for completeness, but the equations are resolved for steady-state conditions. Dirichlet boundary conditions for Y_k and h are imposed in both the reactants and products, where the enthalpy is assigned according to temperature and heat capacity at constant pressure of reactants and products streams, while for K a combination of Dirichlet and Neumann boundary conditions is imposed as follows:

$$\frac{\partial K}{\partial x}(x \to -\infty) = 0, \ \ K(x \to \infty) = a. \tag{2}$$

Lean conditions are established at an equivalence ratio of 0.5 to maximize preferential diffusion effects while not approaching extinctions at high strain rate. Flamelet results with and without preferential diffusion are compared to be able to assess preferential diffusion effects on the flame structure. In the latter case preferential diffusion is thus deliberately suppressed, i.e. $Le = 1$ is assumed for all species. For clarity of treatment, if one tries to isolate preferential and differential diffusion effects (e.g. see [6]), both the effects would be artificially suppressed in the $Le = 1$ case, while both are retained in the multi-component case. Since artificially isolating the two different effects is challenging, the analysis and the conclusions of the present work are mostly focused on preferential diffusion effects (occurring due to hydrogen's higher molecular diffusivity with respect to other species), which are the ones triggering a local change of mixture fraction across the flame (see Section 3.2), and their interplay with strain. Instead, the term “differential” will be used only in the context of diffusive fluxes to highlight a different flux between fuel and oxidizer.

Stretch is defined by the fractional rate of change of a flame surface element propagating in a non-uniform flow, which is caused by the combination of tangential strain rate (a_t) and curvature ($s_d/\mathcal{R}$) effects [23, Chap. 2.6]:

$$\kappa = \frac{1}{A}\frac{dA}{dt} = a_t + \frac{s_d}{\mathcal{R}}. \tag{3}$$

The radius of curvature $\mathcal{R}$ is defined positive (negative) for surface elements that are concave towards the products (reactants) in a premixed flame, and s_d is the displacement speed of the propagating surface element relative to the fresh gases. This study focuses on the strain rate contribution to stretch. In fact, in the investigated stationary and planar 1D configuration, the curvature term is equal to zero and the effect of flame straining can be isolated. There are two related parameters that can identify strain appearing in the governing flamelet equations. The first is represented by the applied strain rate, which is a flamelet setup parameter and is defined as the velocity gradient at the products boundary:

$$a = -\left(\frac{du_x}{dx}\right)_p . \tag{4}$$

The local strain rate in this type of flamelet is instead defined as

$$K(x) = \frac{\partial u_y}{\partial y}, \tag{5}$$

and is introduced in the governing equations to consider the influence of the vertical component of the flow on the transported quantities. From the mass conservation Eq. (1a), the relationship between the two quantities reads $K_{x\to\infty} = a$.

In order to monitor the local leaning and enrichment effect of the flame due to the combination of hydrogen preferential diffusion and strain effects, it is convenient to define the mixture fraction according to Regele et al. [7]. Rearranged for the investigated lean premixed counterflow configuration, the definition reads

$$Z = \frac{\nu Y_{H_2} - Y_{O_2} + Y_{O_2,\mathrm{air}}}{\nu + Y_{O_2,\mathrm{air}}}, \tag{6}$$

where $Y_{O_2,\mathrm{air}}$ is the mass fraction of oxidizer in air and ν is defined as the mass stoichiometric ratio

$$\nu = \frac{\nu_{O_2} W_{O_2}}{\nu_{H_2} W_{H_2}}, \tag{7}$$

with the stoichiometric coefficient of the species k denoted by ν_k.

3. Results and discussion

3.1. Radical peaks trends

The distribution of H radical mass fraction as a function of the flame-centred, flame-thickness-normalized longitudinal flamelet coordinate at different strain rates computed with the multi-component diffusion model and $Le = 1$ are compared in Fig. 2. The flame position at different strain rates is defined as $x_0 = x(c = 0.5)$, where the progress variable c is based on the water mass fraction, $c = \frac{Y_{H_2O}}{Y_{H_2O,\max}}$, and the thermal thickness is taken as flame thickness, $\delta = \frac{T_p - T_r}{|\partial T/\partial x|_{\max}}$. For clarity of treatment, we indicate the flame region where $0.5 < c < 0.9$, and we refer to the preheat and post flame zone where $c < 0.5$ and $c > 0.9$, respectively. The peak of radical concentration is observed to increase with strain rate in the case with preferential diffusion. The same trend is observed for other radicals, such as OH, O and N (not shown), and similar evidence was found also in previous studies [16] at slightly richer conditions. This behaviour is likely to drive the increase of the peak reaction rate and heat release rate with strain [15], and with positive curvature [24,25] in hydrogen flames.

In contrast, when no preferential diffusion effects are taken into account, the flame appears substantially insensitive to strain, as peaks of Y_H remain about constant. Moreover, the peak values in the unitary Lewis number case are higher than the ones of the case with preferential diffusion. This is consistent with the peaks of reaction rate that are also higher in the unitary Lewis number case, as can be observed in Fig. 3. The comparison between Figs. 2 and 3 thus suggests that the high diffusivity of atomic hydrogen is somewhat limiting its burning potential. Despite this, hydrogen's peak reaction rate and heat release rate are still significantly stronger than the ones found in hydrocarbon fuels at similar regimes. This is because the set of chemical reactions that are governing hydrogen combustion is such that more free H radicals are generated than consumed in a reaction step, i.e. the consumption of hydrogen is chain-branching. The further consumption of these radicals is contributing to the total heat release. This is not the case in hydrocarbon fuels, whose consumption is instead chain-breaking.

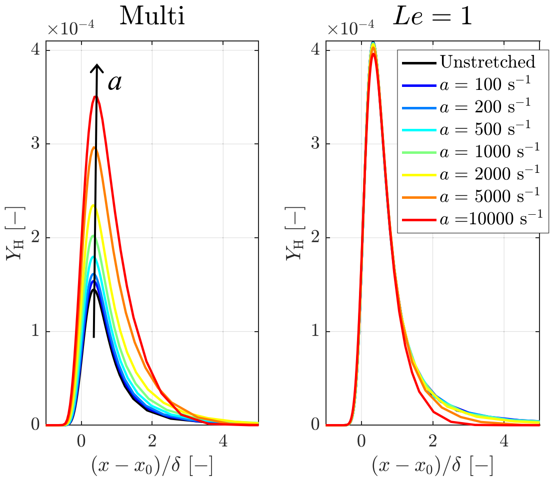

Fig. 2. Distribution of H radicals mass fraction at different strain rates obtained with multi-component diffusion model (left) and $Le = 1$ model (right).

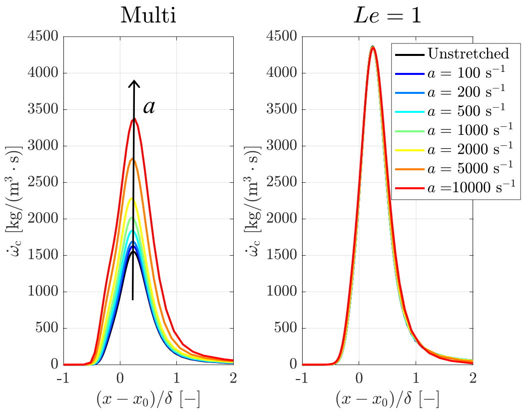

Fig. 3. Distribution of progress variable reaction rate at different strain rates obtained with multi-component diffusion model (left) and $Le = 1$ model (right).

3.2. Mixture fraction distribution

The distribution of the mixture fraction as defined in Eq. (6) across the flamelet, computed with the multi-component and $Le = 1$ diffusion models, is shown in Fig. 4. Without preferential diffusion, the mixture fraction is expected to be constant across the flame, and the flamelet results for the $Le = 1$ case confirm this expectation for any strain level. Only minor local oscillations are visible due to the employed simplified definition of the mixture fraction, and this inaccuracy is addressed in the supplementary material. As suggested in previous studies of unstrained premixed hydrogen flames [7], a local dip (i.e. a local decrease of mixture fraction or equivalently a leaner mixture) can be instead expected when preferential diffusion is present, as the different species molecular diffusivities trigger a local imbalance between fuel and oxidizer. A similar dip to the one observed for unstretched flames can also be recognized for strained flames, as shown in Fig. 4. However, this leaner region is observed to be followed by an overshoot of mixture fraction, and this overshoot becomes stronger as the strain

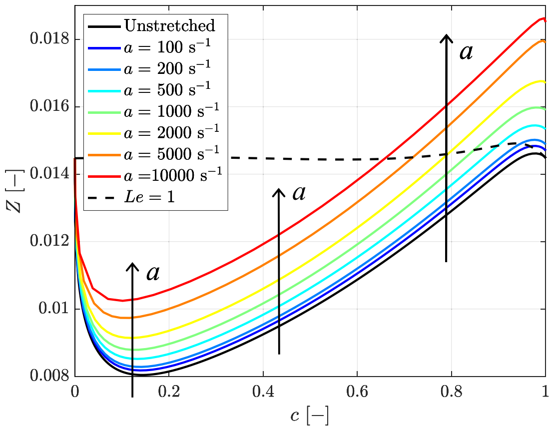

Fig. 4. Distribution of mixture fraction across the flamelet at different strain rates obtained with multi-component (solid lines) and $Le = 1$ (dashed lines) diffusion models.

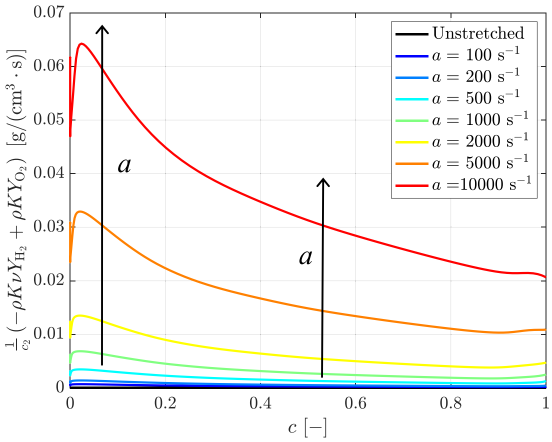

Fig. 5. Differential strain term across the flamelet as defined in Eq. (11) for different applied strain rates.

rate imposed to the flame increases indicating that a local enrichment is experienced by the flame. Similar results were also observed in other works under strained [13] and positively curved conditions [25]. Given that this overshoot is not present in freely propagating unstretched flame configurations, the only possible responsible for this outcome is strain. The local enrichment further leads to super-equilibrium values of the combustion products [13].

It can also be observed from Fig. 4 that the local decrease of mixture fraction is more limited when strain rate is increased. This suggests that strain somewhat limits the local leaning of the flame that occurs because of preferential diffusion, thus smearing its effect on lean premixed hydrogen flames. Overall, this results in a general enrichment of the mixture within the flame front at higher strain rates, see Fig. 4. Note that in absence of preferential diffusion, there is not such influence of strain, as Z is constant across the flame at any strain rate when the species have equal molecular diffusivities. In the next subsection, the reasons behind the mixture fraction response to strain observed are further investigated quantitatively.

3.3. Mixture fraction transport

The transport equation of mixture fraction for a one-dimensional steady counterflow flame is

$$\frac{\partial}{\partial x}\left(\rho u_x Z\right) = -\frac{\partial J_{x,Z}}{\partial x} - \rho K Z, \tag{8}$$

where $J_{x,Z}$ is the diffusive flux of the mixture fraction across the flamelet direction [7]. For simplicity, the analysis is carried on flamelet results obtained with a constant non-unity Lewis number diffusion model (Leconst) and neglecting thermal diffusion effects. Following the methodology of Vance et al. [26], the constant Lewis numbers of each species are obtained by fitting the results of the simulation with the multi-component diffusion model at the same strain rate. The diffusive flux $J_{x,Z}$ in Eq. (8) can be expressed as [7]:

$$\begin{aligned} J_{x,Z} = &-\frac{\lambda}{c_p}\frac{\partial Z}{\partial x} - \frac{\lambda}{c_p}\left(\frac{1}{Le_{H_2}} - 1\right)(1-Z)\frac{\partial Y_{H_2}}{\partial x} \\ &- \frac{\lambda}{c_p} Y_{H_2}\left(\frac{1}{Le_{H_2}} - 1\right)(1-Z)\frac{1}{W}\frac{\partial W}{\partial x}, \end{aligned} \tag{9}$$

where W is the mixture molar mass. Note that the choice of the diffusion model does not alter the trends with strain rate of the flame physical properties observed in previous subsections, and will not thus affect the general conclusions (see also supplementary material). The strain rate term in Eq. (8) can be decomposed as follows

$$-\rho K Z = -\frac{\rho K}{c_2}\left(\nu Y_{H_2} - Y_{O_2} + c_1\right), \tag{10}$$

where $c_1 = Y_{O_2,\mathrm{air}}$ and $c_2 = \nu + c_1$ are both positive constants. Hence, considering the first two terms on the right-hand-side of Eq. (10), a "differential" strain term can be defined as

$$\frac{1}{c_2}\left(-\rho K \nu Y_{H_2} + \rho K Y_{O_2}\right). \tag{11}$$

The differential strain term determines whether the fuel and oxidizer are being transported due to strain in the second dimension of the counterflow following their stoichiometric proportions (for which the differential strain would vanish), or if instead there is an imbalance. An imbalance is eventually what would trigger a local leaning and enrichment of the mixture fraction with changing strain rate. This term is plotted in Fig. 5 across the flamelet at different strain rates. It is visible that the differential strain rate is positive across the progress variable for any flamelet investigated, and with reference to Eq. (11) this implies that

$$-\rho K \nu Y_{H_2} + \rho K Y_{O_2} > 0, \tag{12}$$

and thus that

$$\left|\rho K \nu Y_{H_2}\right| < \left|\rho K Y_{O_2}\right|. \tag{13}$$

Eq. (13) shows that more O_2 is transported in the second dimension by strain than H_2 with respect to the mass stoichiometric proportions for hydrogen combustion. This proves that the conditions for an overall mixture enrichment are established because of the application of strain rate. Furthermore, the figure shows that this effect is amplified when the applied strain rate is increased, because the differential strain term is increasing with applied strain rate, and so is the difference between oxygen and hydrogen being transported in the second dimension (with respect to the stoichiometric case). This is also consistent with the mixture enrichment with strain rate observed in Fig. 4.

In order to further understand the way the mixture fraction is locally affected by combined strain and preferential diffusion effects, the mixture fraction diffusion term is also shown for different strain rates in Fig. 6, where the diffusive flux is computed according to Eq. (9). In the figure, two different regions can be identified. For $c > 0.2$, the diffusion term is positive, which means that the mixture fraction has to increase at this location. Fig. 6 shows that the higher is the strain rate, the stronger in module the diffusion term becomes at the same location, which is due to the fact that species gradients are steepened by strain. Along with the local enrichment enabled by the strain rate, this is probably the reason why strain triggers super-equilibrium values of Z at the products side (see Fig. 4), leading to super-equilibrium products.

In the second region identified in Fig. 6, where $c < 0.2$, the diffusion term is negative at all strain rates, which corresponds to a decreasing

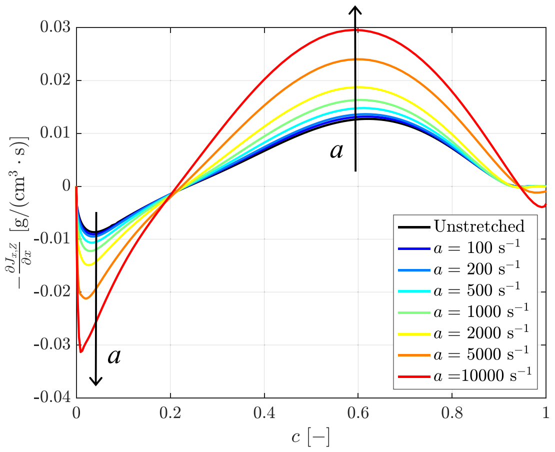

Fig. 6. Mixture fraction diffusion term across the flamelet as defined at the first term at the right hand side in Eq. (8) and by Eq. (9) for different applied strain rates.

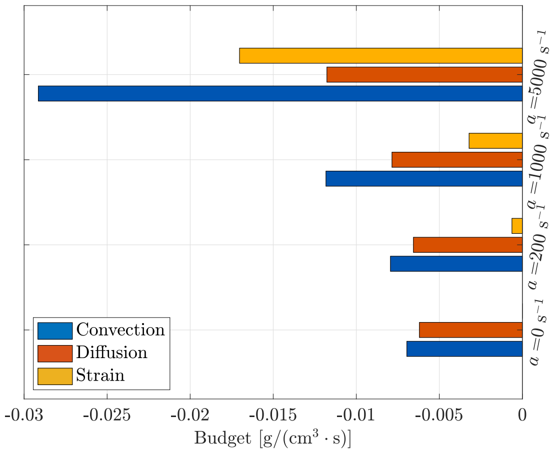

Fig. 7. Bar chart showing the budget terms of Z according to Eq. (8) at c = 0.1 and at four different sample applied strain rates.

mixture fraction, as Z is transported out of this region by diffusion. Furthermore, as the applied strain rate increases, the diffusion term becomes increasingly negative at the same location, which is again due to species gradients being steepened. One could expect that this increase in magnitude should by itself trigger a further local leaning of the burning mixture. However, this is not the case as observed in the plot in Fig. 4, which instead shows that the mixture is enriched by strain rate all across the flamelet. We believe that the reason behind this is that the strain rate term, which triggers an enrichment of the mixture all across the flamelet, overcompensates for the expected leaning of the mixture. This argument is supported by Fig. 5, which shows that the peak of differential strain rate is positioned in the proximity of where the negative peak of diffusion term is found across the flamelet. To further confirm this argument, the budgets of each term in Eq. (8) at $c = 0.1$ are reported in Fig. 7 for increasing applied strain rates. In this figure the sum of the diffusion and strain terms is equal to the convection term (which is the term at the left hand side in Eq. (8)), as one would expect. The figure shows that when the applied strain rate is increased, the relative contribution of the strain rate term in compensating for the convection term also increases with respect to that of the diffusion term. For instance, at $a = 200$ s^{-1}, the strain term contributes only marginally (9%) to balance the convection, with the diffusion term being the main contributor (91%). In contrast, at $a = 5000$ s^{-1}, the situation is inverted with the strain term balancing the 59% of the convection term and the diffusion term contributing for 41%. To summarize, this shows that when the strain rate is increased, two effects occur in this region where $c < 0.2$. On the one hand, the diffusion term's negative peak intensifies, potentially causing the flame to lean locally. On the other hand, the strain term, previously discussed to cause local flame enrichment, increasingly counteracts this effect. Ultimately, the contribution of the strain term overcompensates the effect of the diffusion term and thus triggers an overall local enrichment of the flame. Note that an enrichment is still observed at $a = 1000$ s^{-1} in Fig. 4, and according to Fig. 7 the contribution of strain is still lower than that of diffusion at this value of strain, which seems to contradict the previous discussion. Nevertheless, an increase of the strain term is expected to have a stronger effect on the mixture fraction with respect to a similar increase of the diffusion term. This is because the former is a linear function of Z, while the latter only acts on its second derivative, thus having a less significant effect on Z itself. Note also that the gradients shown in Fig. 7 were computed *a posteriori* and some accuracy error might be expected, although these do not affect the generalities of the discussion above.

3.4. Flame physical properties

In order to draw general conclusions on the mutual effect of strain and preferential diffusion on the global performance of hydrogen flames, the effect of the investigated mixture fraction variation on the flame physical properties is discussed in this subsection. The flame thermal thickness as a function of strain for the two cases with and without preferential diffusion is reported in Fig. 8. As expected, the multi-component unstretched flame is thicker by a factor $Le_{\mathrm{H_2}}^{-1/2}$ [27] with respect to the unstretched $Le = 1$ and this is due to preferential diffusion triggering species redistribution over a wider region at low progress variables, thus relaxing the species gradients across the flamelet. The graph further shows that for both the diffusion models strain reduces the flame thickness due to the stronger flow convection, but that this reduction is steeper in the flamelets computed with the multi-component model. This could be due to the fact that the strain term in the transport equations is becoming more and more dominant with respect to the diffusion term, as also discussed for the mixture fraction in Section 3.3. This means that each fluid element is preferentially being transported in the second dimension (tangentially to the flame) from the strain term rather than being transported in the longitudinal dimension (normal to the flame) by the diffusion term. Hence, preferential diffusion effects, which were smoothing the gradients in unstretched conditions, are now inherently being overcome by strain effects when the applied strain rate is increased. This ultimately explains the steeper flame thickness decrease with strain as compared to the $Le = 1$ case observed in Fig. 8.

The consumption speed is also reported In Fig. 9, defined as $S_c = -\frac{1}{\rho_r Y_{\mathrm{H_2},r}} \int_{-\infty}^{\infty} \dot{\omega}_{\mathrm{H_2}}\, dx$. First of all, it can be seen as expected that the flame speed is lower in the multi-component case compared to the $Le = 1$ case in unstretched conditions because of the mixture being locally leaned by preferential diffusion. Furthermore, the well-known negative hydrogen fuel Markstein length can be immediately observed for the case with preferential diffusion turned on by noticing the increasing consumption speed with strain. Of course, this trend is triggered by the mixture being locally enriched with increasing applied strain rate as discussed in Section 3.2. It is worth noting that despite the overall burning mixture enrichment observed as strain increases, the peak reaction rate does not achieve the (high) values one would obtain when preferential diffusion effects are suppressed, even at relatively high strain levels (see Fig. 3). Nevertheless, due to the combination of thicker flame (see Fig. 8) and enhanced burning rate, the consumption speed for $a > 2000$ s^{-1} reaches values above those one would obtain without taking preferential diffusion into account. This means that the flame performance in terms of consumption speed, initially limited

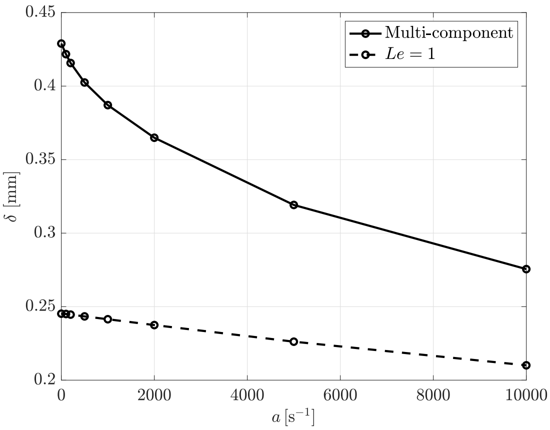

Fig. 8. Evolution of the thermal flame thickness with strain.

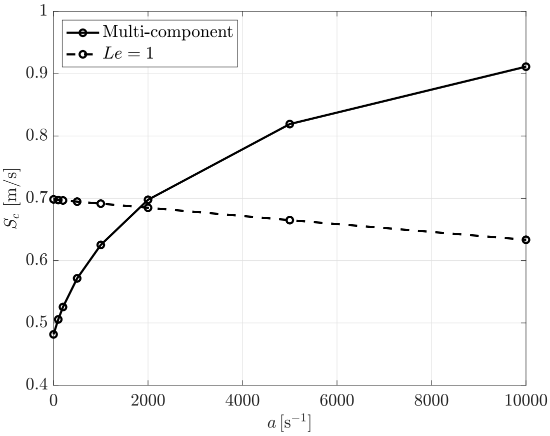

Fig. 9. Evolution of the consumption speed with strain.

by preferential diffusion effects in unstretched conditions due to the flame burning locally leaner, are re-enhanced and even improved by the overall burning mixture enrichment triggered by increasing strain rate.

3.5. Discussion

The analyses in Sections 3.1 and 3.4 have indicated that in presence of preferential diffusion effects, certain flame physical and global properties such as peak reaction rate, peak radical concentration, flame thickness, and consumption speed are suppressed, limiting the burning performance in a lean hydrogen flame. However, when strain rate is applied, these properties are restored towards the levels that one would observe if preferential diffusion effects were artificially turned off. This suggests that mean strain rate can play a role in mitigating the limitations imposed by preferential diffusion effects on the flame behaviour. This observation on the physical properties is quantitatively confirmed by inspecting the budget terms of the mixture fraction, which showed that with increasing applied strain rate an element of fluid is more and more preferentially being transported in the second dimension rather than diffusing across the flamelet longitudinal direction, thus limiting the impact of preferential diffusion effects on the flame itself. Furthermore, fuel and oxidizer are being differentially transported in the second dimension by the strain term such that the burning mixture is enriched. Overall, this results in a mitigation of the flame leaning triggered by preferential diffusion in unstretched conditions, and in a general enrichment of the mixture, which ultimately enables an improvement of the burning performance. Note that the discussed mitigation of preferential diffusion effects by intensive mean applied strain rate can be at first glance linked to a similar mitigation of thermodiffusive instabilities by increasing turbulence level and so Karlovitz number in practical applications. However, it is important to remark that the macroscopic response of the flame to mean strain rate investigated here in laminar conditions should not be confused with the microscopic local flame response to strain due to turbulence, and this is further discussed in Section 5 of the supplementary material.

As final consideration, it was already shown in Berger et al. [13] that the effect of mean positive strain in a lean turbulent hydrogen flame is to steepen scalar gradients, leading to an enhancement of the mean mixture fraction and higher mean reaction rates within the flame. In their study it is concluded that both strain and curvature amplify the effect of preferential diffusion in lean hydrogen flames. In their case, however, the flame is not subject to strong mean tangential gradients, and only experiences local strain and curvature due to turbulence. In light of the analysis presented in this work, and of the broad range of mean strain rate investigated in laminar conditions, it can be rather concluded that mean strain limits the species from differentially diffusing across the flame longitudinal direction, as it instead triggers a preferential species transport on the flame tangential direction. Hence, the way preferential diffusion affects the flame is limited by mean strain, with most of the flame physical properties approaching those one would obtain in the hypothetical case in which preferential diffusion is turned off. By studying laminar bluff body stabilized premixed hydrogen flames, Vance et al. [17] further highlighted that in correspondence of highly stretched regions, the flame stabilizes beyond the lean flammability limit. This phenomenon was generically linked to “stronger preferential diffusion effects”, in light of an observed higher elemental hydrogen mass fraction. The findings presented in this study suggest, however, that while the delayed lean blow off is indeed caused by the strengthening of the flame as consequence of the higher local stretch, this phenomenon is due to the species differential diffusive fluxes becoming less significant to the overall species transport, rather than becoming more dominant.

4. Conclusions

Detailed chemistry one dimensional simulations have been conducted on pure hydrogen lean premixed strained flamelets for a broad range of strain rates. Preferential diffusion was turned on and off in the modelling in order to highlight its effect on the flame structure and its interplay with the strain effects. The analysis shows for the first time that strain has a mitigating effect on the importance of fluid elements cross-flame diffusion, as they are preferentially being transported on the vertical or flame-tangential direction. This phenomenon has the effect of limiting the weakening impact of fuel/oxidizer differential diffusive fluxes on the flame physical properties and burning performance, which are a consequence of a leaner burning mixture at unstretched conditions, by triggering a global flame enrichment. This finding contradicts previous studies where stretch was generally indicated to enhance the effects of preferential diffusion on the flame. Future work will focus on expanding the analysis to a two-dimensional setup to explore the combined effect of tangential strain rate and local curvature. In particular, the present one-dimensional study suggests that intensive mean applied strain rate may somewhat limit the propagation of thermodiffusive instabilities (triggered by locally curved flame fronts) by establishing a transport of fluid elements in the flame tangential direction which can be significantly stronger than the fluid elements diffusion across the flame normal direction.

Novelty and significance statement

The novelties of this study are summarised below:

- This study thoroughly investigates on the combined effect of intensive applied strain rate and preferential diffusion in lean hydrogen flames for the first time.
- Unlike previous studies attributing to strain an enhancing influence on preferential diffusion, this work proposes an opposite interpretation, where strain progressively mitigates the impact of the differential diffusive fluxes between fuel and oxidizer across the flame normal direction.
- A budget analysis of the transport terms of mixture fraction is performed for the first time to assess the relative importance of fuel/oxidizer cross-flame differential diffusive fluxes and of their differential transport in the second dimension due to increasing strain rate.

CRediT authorship contribution statement

Alessandro Porcarelli: Designed the research analysis on mutual effect of strain and preferential diffusion, Performed the analyses, Drafted the paper. **Ivan Langella:** Initiated the research topic, Revised the draft, Contributed to results interpretation, Supervised the research.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.proci.2024.105728.

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