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A study of flame dynamics and structure in premixed turbulent planar $NH_3/H_2/air$ flames

Parsa Tamadonfar^{*a*,*}, Shervin Karimkashi^{*a*}, Ossi Kaario^{*a*}, Ville Vuorinen^{*a*}

^aDepartment of Mechanical Engineering, School of Engineering, Aalto University, Otakaari 4, Espoo 02150, Finland

Abstract

Ammonia (NH₃) has received considerable attention as a near future carbon-free synthetic fuel due to its economic storage/transportation/distribution, and its potential to be thermally decomposed to hydrogen (H₂). To promote the low burning velocity and heat of combustion of ammonia, one viable option is to enrich pure ammonia with hydrogen. In this study, two quasi direct numerical simulations (quasi-DNS) with detailed chemistry and the mixture-averaged transport model are examined to study stoichiometric planar ammonia/hydrogen/air flames under decaying turbulence. The reactants temperature and pressure are set to 298 K and 1 atm, respectively. The initial turbulent Karlovitz number is changed from 4.3 to 16.9, implying that all the test conditions are located within the thin reaction zones combustion regime. The results indicate that the density-weighted flame displacement speed (S_d^*), on average, is higher than the unstrained premixed laminar burning velocity (S_L^0) value for both test cases. This suggests that the flame elements propagate faster than their laminar flame counterpart. With increasing the Karlovitz number, the turbulent burning velocity and the wrinkled flame sur-

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face area increase by about 35%. Furthermore, the mean flame stretch factor defined as the ratio of the turbulent to the laminar burning velocity divided by the ratio of the wrinkled to the unwrinkled flame surface area is equal to 1.08. This indicates that the local flamelet velocity value, on average, is higher than the unstrained premixed laminar burning velocity. In addition, the results show that the mean value of the local equivalence ratio for the turbulent conditions is higher than its laminar counterpart due to the preferential diffusion of hydrogen and turbulent mixing. Furthermore, the net production rate of hydrogen is shown to be negatively correlated with the flame front curvature suggesting that the local burning rate is intensified in positively curved regions.

Keywords:

Premixed turbulent flames, Ammonia, Hydrogen, Quasi direct numerical simulation, Flame displacement speed

1. Introduction

Increasing the efficiency of combustion devices as well as using novel carbonfree synthetic fuel blends are considered the main targets to decrease greenhouse gas emissions. One of the suitable options for attaining this target is to utilize hydrogen produced from green-energy origins. However, the economic storage and transportation of hydrogen have not been resolved very well [1]. Therefore, the operation of combustion devices running on pure hydrogen is still a matter of ongoing research. Among all hydrogen carriers, ammonia has received substantial attention as a carbon-free fuel due to its high energy density; and its transportation, storage, handling, and distribution have been very well established [1, 2]. It should be noted that since the condensation pressure and boiling temperature of ammonia are relatively similar to those of propane, ammonia transportation may not pose significant challenges for transport ships [2]. However, the main disadvantages of using pure ammonia as a main fuel are its low laminar burning velocity and heat of combustion [1]. It should be mentioned that increasing the reactivity of pure ammonia could be done by enriching it with hydrogen and/or oxygen. Figure 1 shows the variation of the heat release rate with respect to the flame temperature for 1-D premixed laminar ammonia/air, ammonia/hydrogen/air with a blending ratio of 0.4, and methane/air flames. The blending ratio is defined as the amount of hydrogen concentration in the ammonia/hydrogen mixture. For these 1-D simulations, the equivalence ratio values for the ammonia/air, ammonia/hydrogen/air, and methane/air flames are equal to 1.0, 1.0, and 0.85, respectively. The reactants temperature is equal to 298 K and the pressure is set to 1 atm in these cases. These three numerical simulations are performed using Cantera, which is an open-source chemical kinetics software. The results presented in Fig. 1 show that the heat release rate of pure ammonia is quite negligible compared to the methane/air flame, and enriching it with 40% of hydrogen could have a significant impact on its value. With adding hydrogen, the heat release rate value of the ammonia/hydrogen/air mixture is comparable with the methane/air mixture. Since ammonia has the capability to be thermally decomposed on-board to ammonia and hydrogen, studying the characteristics of ammonia and hydrogen blends is of particular interest.

Despite the active research in using novel fuel blends for premixed turbulent combustion, there still exist many unsolved problems for such flames. Among different flame properties, flame speed is one of the important characteristics for premixed turbulent flames, and comprehending the behaviour of this property is



Figure 1: Heat release rate with respect to the temperature for 1-D premixed laminar ammonia/air, ammonia/hydrogen/air with a blending ratio of 0.4, and methane/air flames. The equivalence ratios for ammonia/air, ammonia/hydrogen/air, and methane/air flames are set to 1.0, 1.0, and 0.85, respectively. The reactants temperature is equal to 298 K and the pressure is set to 1 atm. The simulations are performed using Cantera, which is an open-source chemical kinetics software.

required for the flamelet modeling [3]. The flame displacement speed, the turbulent burning velocity, and the local consumption speed are among the important flame characteristics in flame speed modeling, and understanding the behaviour of these parameters is required for less explored novel fuel blends such as ammonia/hydrogen/air flames under different turbulent conditions.

The local turbulence-chemistry interactions could be understood in depth by knowing the flame displacement speed (S_d) characterizing the speed of an iso-scalar surface relative to the flow field [4, 5, 6]. It should be noted that the flame displacement speed has been the subject of various numerical studies. Peters et

al. [4] and Echekki and Chen [5] discussed the contributions of the flame front curvature on the flame displacement speed components using direct numerical simulation (DNS) of a 2-D methane/air flame. Chakraborty and Cant [7] showed that the flame displacement speed is negatively correlated with the flame front curvature using 3-D DNS with simple chemistry, which is consistent with other studies reported in Refs. [4, 5]. Song et al. [6] analysed the density-weighted form of the flame displacement speed for highly turbulent hydrogen/air flames, and they concluded that the most probable values of the local flame displacement speed are relatively equal to the unstrained premixed laminar flame. Chakraborty and Cant [8] discussed the influence of the Lewis number on the flame displacement speed statistics based on 3-D DNS with simple chemistry. They showed that the flame displacement speed, irrespective of the Lewis number, is negatively correlated with the flame front curvature, and the density-weighted flame displacement speed is higher than the unstrained premixed laminar burning velocity when the Lewis number is less than unity. More recently, Chakraborty et al. [9] assessed the performance of various extrapolation relations connecting the density-weighted flame displacement speed to the flame front curvature and flame stretch rate for thermo-diffusively neutral flames using 3-D DNS with detailed chemistry, since the accurate modeling of this quantity is required for the closure of the flame surface density transport equation. They showed that the density-weighted flame displacement speed could be evaluated using the linear model based on the flame front curvature in a very robust manner.

In addition to the flame displacement speed, the turbulent burning velocity $(S_{\rm T})$ is considered an important parameter for premixed turbulent combustion. It should be kept in mind that many attempts have been done over several decades to

correlate the turbulent burning velocity data obtained from experimental measurements in terms of various parameters such as the turbulence intensity and turbulent length scale [10, 11, 12]. Damköhler [13] hypothesized that turbulence is responsible for wrinkling the flame front, and the local flamelet consumption velocity is equal to the unstrained premixed laminar burning velocity. According to this hypothesis, the ratio of the turbulent burning velocity to the unstrained premixed laminar burning velocity is equal to the ratio of the wrinkled to the unwrinkled flame surface area. It should be emphasized that the validity of this hypothesis is confirmed based on 2-D and 3-D DNS with simple/detailed chemistry for thermodiffusively neutral flames (unity Lewis number), see, e.g., Hawkes and Chen [3], Han and Huh [14], Nivarti and Cant [15], Klein et al. [16], Brearley et al. [17], and Song et al. [6]. However, this hypothesis might be no longer valid for thermodiffusively unstable flames. Chakraborty et al. [18] showed that the ratio of the turbulent to the laminar burning velocity is higher than the ratio of the wrinkled to the unwrinkled flame surface area for thermo-diffusively unstable flames. A similar observation was previously reported by Han and Huh [14] as well using 3-D DNS with simple chemistry. It should be mentioned that Gülder [19] and Tamadonfar and Gülder [20] discussed that the validity of this hypothesis might be disputed under certain experimental conditions for premixed turbulent Bunsentype flames. More recently, Chakraborty et al. [21] showed that this hypothesis might become invalid for flames with high non-zero mean flame front curvature such as the Bunsen-type flames.

Furthermore, in their comprehensive review paper, Lipatnikov and Chomiak [22] discussed thoroughly the local structure of premixed turbulent flames. They mentioned that the local burning velocity values in positively curved zones are

higher than the corresponding values in negatively curved regions when the Lewis number is less than unity and/or the mass diffusivity of the deficient reactants is higher than the mass diffusivity of the excess reactants. Rutland and Trouvé [23] and Haworth and Poinsot [24] showed a strong correlation between the local burning velocity and the flame front curvature for non-unity Lewis number flame conditions using simple chemistry. Bell et al. [25] reported a positive (negative) correlation between the local burning velocity and the flame front curvature for a premixed turbulent hydrogen/air (propane/air) flame indicating enhanced fuel consumption rate in positive (negative) curvature regions using 2-D DNS with detailed chemistry. They attributed this observation to the thermo-diffusive instability (stable) characteristics of the hydrogen/air (propane/air) flames. Day et al. [26] and Aspden [27] demonstrated a similar correlation between the local burning velocity and the flame front curvature for premixed turbulent lean hydrogen/air flames. More recently, Lee et al. [28] and Rieth et al. [29] showed a positive correlation between the fuel consumption rate and the flame front curvature for highly turbulent premixed lean H_2/air and $NH_3/H_2/N_2/air$ flames developing in a forced turbulence and in a turbulent shear layer, respectively.

To the best of the authors' knowledge, certain aspects of premixed turbulent ammonia/hydrogen/air flames such as the flame displacement speed statistics, the turbulent burning velocity, and the local burning velocity of these flames have been less explored. Therefore, the current study seeks to address these fundamental properties using quasi direct numerical simulation (quasi-DNS) with detailed chemistry. Furthermore, the mixture-averaged transport model is utilized in order to take into account the preferential diffusion of high/low diffusivity species accurately. In this respect, the main objectives of the current work are (1) to study the flame displacement statistics, (2) to explore the turbulent burning velocity and the validity of the Damköhler's first hypothesis, and (3) to discuss the local structure of premixed turbulent planar ammonia/hydrogen/air flames. The remainder of the paper is organized as follows. The numerical methods will be discussed in Sect. 2. This will be followed by results and discussion in Sect. 3, and the concluding remarks in Sect. 4.

2. Numerical methods

2.1. Flame configuration

In this study, quasi direct numerical simulations (quasi-DNS) for premixed turbulent ammonia/hydrogen/air flames have been performed under the global equivalence ratio of unity. It should be noted that OpenFOAM does not provide higher-order discretization schemes unlike other CFD codes developed explicitly for DNS studies. To acknowledge this difference, the term quasi-DNS, used by Zirwes et al. [30] and others, is utilized in this study. The blending ratio (α) indicating the amount of hydrogen concentration in the ammonia/hydrogen mixture is evaluated as $X_{\rm H_2}/(X_{\rm H_2} + X_{\rm NH_3})$, where $X_{\rm H_2}$ and $X_{\rm NH_3}$ are the mole fractions of hydrogen and ammonia, respectively. For the current study, the blending ratio is set to 0.4. The reactants temperature ($T_{\rm r}$) and pressure (p) are set to 298 K and 1 atm, respectively. The unstrained premixed laminar burning velocity ($S_{\rm L}^0$) and the thermal flame thickness ($\delta_{\rm T}$) evaluated based on the maximum temperature gradient are equal to 30.37 cm/s and 0.604 mm, respectively. The adiabatic flame temperature ($T_{\rm ad}$) of this particular mixture is then equal to 2146 K.

The Passot-Pouquet spectrum [31] is utilized for generating the homogeneous isotropic turbulent flow field on a cube with a domain size of $45\delta_T \times 7\delta_T \times$

 $7\delta_{\rm T}$. The Python script used for generating the turbulent flow field was originally developed by Saad et al. [32], and they later added the aforementioned spectrum to their script. The non-dimensional turbulence intensity $(u'/S_{\rm L}^0)$ is varied from 4 to 10, and the non-dimensional integral length scale $(\Lambda/\delta_{\rm T})$ is fixed to 3.5. The domain has been discretized on a uniform Cartesian grid of $990 \times 154 \times 154$ and $1100 \times 172 \times 172$ cells for the low and high turbulence intensity test cases, respectively. Flame-turbulence interactions happen under decaying turbulence. It should be emphasized that such turbulence characteristics without active turbulence generation are essential in the internal combustion engines context. The turbulent flow field is then superimposed on a solution of 1-D unstrained premixed reference laminar flame. The grid spacing ensures that at least 22 computational data points exist within the flame thickness, and the initial Kolmogorov length scale ($\eta \approx \Lambda Re_{\Lambda}^{-3/4}$) resides within one computational cell, where Re_{Λ} is the turbulent Reynolds number. The turbulent Reynolds number (Re_{Λ}) , Karlovitz number (Ka), and Damköhler number (Da) are estimated as $u'\Lambda/\nu$, $(u'/S_{\rm L}^0)^{1.5} (\Lambda/\delta_{\rm T})^{-0.5}$, and $\Lambda S_{\rm L}^0/u'\delta_{\rm T}$, respectively. The effective Lewis number, using the methodology presented in Ref. [33], is equal to 0.76 for both cases implying that the test cases are thermo-diffusively unstable. Table 1 shows the simulation parameters for the test conditions utilized in this study. Figure 2 shows that all the test conditions studied in this work lie within the thin reaction zones combustion regime since the initial Karlovitz number is higher than unity.

2.2. Reactive Flow Solver

The open-source C++ CFD toolbox OpenFOAM [36], where mass, momentum, species mass fractions, and energy equations are solved with the compressible PIMPLE algorithm is utilized to perform quasi-DNS with detailed chemistry



Table 1: Simulation parameters examined in this study.

Figure 2: Numerical data on a Borghi-Peters regime diagram for premixed turbulent combustion regime [34, 35].

for premixed turbulent planar $NH_3/H_2/air$ flames. The chemical kinetic mechanism developed by Stagni et al. [37] consisting of 31 species and 203 reactions is

used in this study. The reactingDNS solver where the mixture-averaged transport model is used to consider the mass diffusivity of each species evaluated from the binary diffusion coefficients is utilized in this study. The successful implementation of this solver was previously shown in Refs. [38, 39, 40, 41, 42]. This approach leads to more accurate results compared to the unity/non-unity Lewis number assumption when simulating the mixtures having high mass diffusivity species such as molecular/atomic hydrogen. It should be emphasized that Aspden et al. [43] noted that the Soret effect is able to shift the quantitative behaviour of lean premixed hydrogen/air flames slightly. However, this effect is not responsible for any qualitative switch for such flames. As a result of this observation, the Soret effect is also ignored in the numerical simulations performed herein for the sake of simplicity. The reactingDNS solver is then linked to the open-source library of pyJac, developed by Niemeyer et al. [44]. This library provides C subroutines for generating the analytical Jacobian of a chemical kinetic mechanism which is required for solving a system of ordinary differential equations. The operator-splitting approach is utilized considering the large differences between the chemistry and flow time scales. It should be emphasized that to overcome the computational load imbalance among processors originating from the chemistry problems, a dynamic load balancing model (DLBFoam), developed by Tekgül et al. [45], is used to distribute the chemistry problems equally among all processors using the MPI communication protocol. This model was previously used for studying spray-assisted dual-fuel ignition [46, 47], spray-assisted tri-fuel ignition [48], and premixed turbulent flame propagation [49].

Inflow and outflow boundary conditions with a zero mean inlet velocity in the direction of the mean flame propagation are used. In the lateral direction, the

periodic boundary conditions are employed, indicating an unbounded planar flame brush. For pressure, a non-reflecting boundary condition is applied for both inflow and outflow regions. A second-order implicit backward Euler method for time discretization and the cubic scheme for spatial discretization have been utilized herein. The simulation runs for 2 (2.85) initial eddy turn-over times for case L (M) ensuring that the simulation time is equal/higher than the chemical time scale. The eddy turn-over time ($t_{\rm e}$) and the chemical time scale ($t_{\rm chem}$) are evaluated as Λ/u' and $\delta_{\rm T}/S_{\rm L}^{\rm 0},$ respectively. Figure 3 shows an example of an instantaneous flame front surface, the cut plane of a temperature field, and the logarithm of enstrophy values for cases L and M. The magnitude of the enstrophy is evaluated as $0.5 |\nabla \times \vec{u}|^2$, where \vec{u} is the local fluid flow velocity. It should be noted that the enstrophy values for case M are higher than case L because of higher turbulence intensity. Furthermore, Fig. 4 shows the Lewis number (Le) fields of ammonia (NH₃), molecular hydrogen (H₂), atomic hydrogen (H), and water (H₂O). The Lewis number for each species (Le_j) is evaluated as α_t/D_j , where $\alpha_{\rm t}$ and D_j are the thermal diffusivity of the mixture and the mass diffusivity of species j, respectively. The results show that the variation of the Lewis number value across the flame brush is insignificant for NH₃, H₂, and H, while it varies significantly for H₂O. A similar observation was shown by Poinsot and Veynante [50].

3. Results and discussion

Before examining a quantitative analysis on premixed turbulent $NH_3/H_2/air$ flame dynamics, a general overview of flame characteristics will be provided. Later in this section, the conditional mean profiles of major species and the atomic



Figure 3: Instantaneous flame front surface, cut plane of a temperature field, and the logarithm of enstrophy for (a) case L, and (b) case M.



Figure 4: Lewis number fields for (a) ammonia (NH₃), (b) molecular hydrogen (H₂), (c) atomic hydrogen (H), and (d) water (H₂O) for case M. These data are captured at 2.85 initial eddy turn-over times. The unburned (burned) region is located on the left (right).

hydrogen, the flame displacement speed statistics, the mean flame stretch factor and the turbulent burning velocity, the local equivalence ratio, and the molecular diffusion fluxes of molecular/atomic hydrogen will be discussed. This will be followed by inspecting the fuel net production rate over the curved flame fronts.

3.1. General overview of flame characteristics

Figure 5 shows the two-dimensional slices of temperature and enstrophy, and Figure 6 presents the mass fractions of H₂O₂, HNO, NH species, and heat release rate for cases L and M. The solid lines (from left to right) correspond to the temperature-based reaction progress variable (c) values of 0.1, 0.2, 0.5, 0.7, and 0.8, where c is evaluated as $(T - T_r) / (T_{ad} - T_r)$. From the visual inspection of the temperature field, the flame wrinkling, preheat zone layer, and possibly the flame surface area increase with increasing the Karlovitz number. This could be due to the existence of higher enstrophy magnitudes, i.e., stronger turbulence structures, in the preheat zone layer for case M compared to case L. The results indicate that the enstrophy values have damped significantly in the reaction zone layer, i.e., c = 0.8, due to the existence of the high heat release region. Therefore, the reaction zone layer is not disrupted for both test cases. It should be emphasized that the mass fractions of H_2O_2 and HNO are the proper markers for the preheat and reaction zone layers for this particular mixture, respectively, since the maximum value of the former (latter) species happens in the preheat (reaction) zone layer as shown in Fig. 7 for a premixed laminar ammonia/hydrogen/air flame with a blending ratio of 0.4. Furthermore, our current results in Fig. 6 indicate that the mass fraction distribution of H_2O_2 is disrupted dramatically with increasing the Karlovitz number indicating the local broadening of the preheat zone layer. This broadening is also noticeable by looking at the temperature-based reaction progress variable iso-lines shown in Fig. 6. In addition, the mass fraction distribution of HNO is not altered implying that the reaction zone layer remains relatively intact. Furthermore, the results show that the distribution of the NH mass fraction coincides with the distribution of the heat release rate.



Figure 5: Two-dimensional slices of temperature and enstrophy for case L (left) and case M (right) from the entire computational domain. The solid lines (from left to right) correspond to the temperature-based reaction progress variable values of 0.1, 0.2, 0.5, 0.7, and 0.8.

3.2. Conditional mean profiles

The conditional mean profiles provide practical information when comparing direct numerical simulations, large eddy simulations, and experiments, and evaluating these profiles gives more insight than analysing the mean concentration profiles [51]. Figure 8 shows the conditional mean profiles of major species and the atomic hydrogen for cases L and M as well as the unstrained premixed refer-



Figure 6: Two-dimensional slices of mass fractions of H_2O_2 , HNO, NH species, and heat release rate for case L (left) and case M (right). The solid lines in the first two rows (from left to right) correspond to the temperature-based reaction progress variable values of 0.1, 0.2, 0.5, 0.7, and 0.8. The whole computational domain is not shown here. The unburned (burned) region is located on the left (right).



Figure 7: Heat release rate and mass fractions of H_2O_2 and HNO with respect to the temperaturebased reaction progress variable for 1-D premixed laminar ammonia/hydrogen/air flame with a blending ratio of 0.4. The equivalence ratio is equal to 1.0. The reactants temperature and pressure are set to 298 K and 1 atm, respectively. These profiles have been normalized by their maximum value.

ence laminar flame. Each profile has been normalized by the maximum value of the corresponding species obtained from the reference laminar flame. The results indicate that the conditional mean profiles of NH_3 and H_2O for the turbulent cases bear a good resemblance to the counterpart profiles of the reference laminar flame. However, the conditional mean profiles of H_2 and H deviate from the premixed laminar flame profiles. This deviation could be due to both the turbulent mixing and preferential diffusion, as discussed thoroughly by Aspden et al. [43]. A similar observation was previously reported by Aspden et al. [52] and Song et al. [6] for highly turbulent premixed hydrogen/air flames propagating in the forced tur-

bulence. Furthermore, it should be noted that the observed deviation for H_2 and H profiles is enhanced with increasing the Karlovitz number. This enhancement could be due to the turbulent mixing weakening the effect of preferential diffusion for high diffusivity species such as H_2 and H.



Figure 8: Conditional mean profiles of NH_3 , H_2O , H_2 , and H mass fractions (solid lines) compared to the unstrained premixed laminar profiles (dashed lines) for (a-b) case L, and (c-d) case M. Each profile has been normalized by the maximum value of the reference laminar flame. The dashed lines correspond to the laminar flame, and the solid lines correspond to the turbulent conditions.

3.3. Flame displacement speed

As mentioned earlier in the Introduction, the flame displacement speed (S_d) which is the flame speed relative to the local fluid velocity is an important flame property, and it is extensively utilized for modeling the turbulent premixed flames using the flame surface density and G-equation models [50, 53]. Following the methodology presented in Refs. [54, 4, 5, 55], the flame displacement speed (S_d) and its components could be estimated as follows:

$$S_{\rm d} = S_{\rm d,r} + S_{\rm d,n} + S_{\rm d,t} = \frac{\dot{\omega}}{\rho \left|\nabla c\right|} + \frac{n \cdot \nabla \left(\rho D n \cdot \nabla c\right)}{\rho \left|\nabla c\right|} - 2D\kappa, \tag{1}$$

where $S_{d,r}$, $S_{d,n}$, $S_{d,t}$, $\dot{\omega}$, n, ρ , D, and κ are the reaction component of S_d , normal diffusion component of S_d , tangential diffusion component of S_d , reaction rate of the reaction progress variable, normal vector to the iso-surface, density, progress variable diffusivity, and the flame front curvature, respectively. The normal vector (n) and the flame front curvature (κ) are evaluated as $-\nabla c/|\nabla c|$ and $0.5 (\nabla .n)$, respectively. It should be noted that in order to compare the flame displacement speed values in a meaningful manner, evaluating the density-weighted form of this quantity is of great importance [5, 6, 55]. As discussed by Song et al. [6], the velocity acceleration across the flame brush originated due to the thermal expansion is excluded by using the density-weighted form of the flame displacement speed (S_d^*) evaluated as:

$$S_{\rm d}^* = \frac{\rho S_{\rm d}}{\rho_{\rm r}},\tag{2}$$

where ρ_r is the reactants density. Each of the flame displacement speed components could be written in their density-weighted format by multiplying their values by ρ/ρ_r . Figure 9 shows the probability density functions (PDFs) of the

density-weighted forms of the flame displacement speed and its components for cases L and M. Each component has been normalized by the unstrained premixed laminar burning velocity of the reference flame, and the data are conditioned at c = 0.8. The results show that the distribution of $S_{\rm d}^*$ and its components widen with increasing the Karlovitz number. A similar observation was previously reported by Song et al. [6] for premixed turbulent hydrogen/air flames. It should be noted that all $S^*_{\rm d}$ values are positive implying that these iso-surfaces move towards the reactants, and its value, on average, is higher than the laminar flame velocity. This deviation from the laminar burning velocity could be due to the preferential diffusion effect. Furthermore, the results show that $S_{d,n}^*$ ($S_{d,n}^*$) are positive (negative) within the reaction zone layer. A similar observation was previously reported for both the density-weighted and density-unweighted forms in the literature, see e.g. Ref. [56, 57]. It should be added that the negative values for $S_{d,n}^*$ do not occur when conditioning the data near the preheat zone layer (not shown). In addition, it should be noted that the highest probability of $S^*_{\rm d,t}$ occurrence happens around zero for both turbulent test cases studied herein.

Furthermore, the joint probability density functions (PDFs) of the densityweighted flame displacement speed with respect to the flame front curvature for both turbulent cases are shown in Fig. 9(e-f). The density-weighted flame displacement speed has been normalized by the unstrained premixed laminar burning velocity, and the flame front curvature has been normalized by the laminar thermal flame thickness. The data are conditioned at c = 0.8. The results show that S_d^* is negatively correlated with the flame front curvature, which is in agreement with previous studies, see e.g., Echekki and Chen [5] for 2-D DNS with detailed chemistry, or Chakraborty and Cant [8] for 3-D DNS using simple chemistry. Furthermore, increasing the turbulence intensity results in generating the flame front with smaller radii, i.e., larger flame front curvature, and the variation of S_d^* promotes significantly. It should be noted that the negative correlation observed between the density-weighted flame displacement speed and the flame front curvature is not sensitive to the selection of the progress variable utilized for conditioning the data (not shown for the sake of brevity). As mentioned earlier, Chakraborty et al. [9] assessed the performance of different extrapolation relations connecting the density-weighted flame displacement speed to the flame front curvature and flame stretch rate using 3-D DNS with detailed chemistry for thermo-diffusively neutral flames. They showed that S_d^* has a negative correlation with the flame front curvature for all their test cases. It should be emphasized that the observed trend in Fig. 9 suggests that this negative correlation remains valid for thermo-diffusively unstable flames using detailed chemistry and the mixture-averaged transport model as well.

3.4. Mean flame stretch factor

Assessing the validity of the Damköhler's first hypothesis is of crucial importance for novel fuel blends such as ammonia/hydrogen/air flames. As mentioned earlier, Damköhler [13] hypothesized that the ratio of the turbulent burning velocity to the unstrained premixed laminar burning velocity (S_T/S_L^0) is equal to the ratio of the wrinkled flame surface area to the unwrinkled flame surface area (A_T/A_L) . This means that the local flamelet velocity (S'_L) is equal to the unstrained premixed laminar burning velocity (S_L^0) . To examine the validity of this hypothesis, the mean flame stretch factor (I_0) could be used as follows [58]:

$$I_0 = \frac{S_{\rm T}/S_{\rm L}^0}{A_{\rm T}/A_{\rm L}},$$
(3)



Figure 9: (a-d) Probability density functions (PDFs) of the density-weighted flame displacement speed and its components for cases L and M. (e-f) The density-weighted flame displacement speed with respect to the flame front curvature for cases L and M. All statistics are conditioned at c = 0.8. The flame displacement speed and its components have been normalized by the unstrained premixed laminar burning velocity, and the flame front curvature has been normalized by the thermal flame thickness.

where $S_{\rm T} = \int_V \dot{\omega} dV / \rho_{\rm r} A_{\rm L}$ and $A_{\rm T} = \int |\overline{\nabla c}| dV$ are the turbulent burning velocity and the wrinkled flame surface area, respectively. The unwrinkled flame surface area ($A_{\rm L}$) is the cross-sectional area normal to the direction of mean flame propagation. It should be noted that the Damköhler's first hypothesis is valid when the mean flame stretch factor value is equal to unity.

The values of the ratio of the turbulent to the laminar burning velocity, the ratio of the wrinkled to the unwrinkled flame surface area, and the mean flame stretch factor are shown in Table 2. The results show that the turbulent burning velocity and the wrinkled flame surface area increase by about 35% with increasing the Karlovitz number. This could be due to the enhancement of flame surface area due to the turbulent structures. A similar observation was previously reported in numerous works in the literature, see, e.g., Han and Huh [14], Nivarti and Cant [15], and Song et al. [6]. Furthermore, the mean flame stretch factor values are shown to be higher than the unity value for both test cases indicating that the mean flamelet consumption velocity is higher than the unstrained premixed laminar burning velocity for ammonia/hydrogen/air flames. This suggests that the Damköhler's first hypothesis is not valid for these test cases. A similar observation was previously reported in the literature for thermo-diffusively unstable flames based on 3-D DNS with simple chemistry, see, e.g., Han and Huh [14], and Chakraborty et al. [18]. As a remark, increasing the turbulence intensity does not have any effect on the mean flame stretch factor values for the cases studied herein.

It should be noted that the local flamelet burning velocity is dependent on the local equivalence ratio across the flame brush [26, 59]. The local equivalence ratio (ϕ) for this particular mixture is evaluated as $0.5 (Z_F/Z_O)$, where Z_F and Z_O are evaluated as $3X_{\rm NH_3} + 2X_{\rm H_2} + X_{\rm H} + X_{\rm OH} + X_{\rm HO_2} + 2X_{\rm H_2O_2} + 2X_{\rm H_2O}$ and $2X_{\rm O_2} + X_{\rm H_2O} + X_{\rm O} + X_{\rm OH} + 2X_{\rm HO_2} + 2X_{\rm H_2O_2} + X_{\rm NO}$, respectively, where X_j corresponds to the mole fraction of species j.

The variation of the local equivalence ratio with respect to the progress vari-

Table 2: The ratio of the turbulent burning velocity to the laminar burning velocity, the ratio of the wrinkled flame surface area to the unwrinkled flame surface area, and the mean flame stretch factor values.

Case	L	М
$S_{\mathrm{T}}/S_{\mathrm{L}}^{0}$	1.444	2.271
$A_{\rm T}/A_{\rm L}$	1.333	2.097
I_0	1.083	1.083

able for the turbulent cases as well as the reference laminar flame is shown in Fig. 10(a-b). The dashed line corresponds to the local equivalence ratio for the laminar flame, and the solid line shows the mean value of the local equivalence ratio for the turbulent conditions. The local equivalence ratio is equal to the global equivalence ratio of unity on the unburned and burned regions, and it decreases from the unity value across the flame brush. It could be seen that the mean local equivalence ratio values deviate from their laminar counterparts for the turbulent cases. This deviation could be attributed to the enhancement of molecular/atomic hydrogen mass fractions due to the turbulent mixing and preferential diffusion effect, as discussed thoroughly by Aspden et al. [43], and it could be the underlying reason why the mean flame stretch factor differs from the unity value. Furthermore, this deviation promotes by increasing the turbulence intensity due to the turbulent mixing weakening the effect of preferential diffusion. It should be emphasized that the local equivalence ratio varies under curved flame fronts, and understanding its characteristics is of great interest since the local flamelet burning velocity is then affected under curved regions. Figure 10(c-d) shows the joint PDFs of the local equivalence ratio with respect to the normalized flame front curvature for both turbulent cases. In this Figure, the flame front curvature has been normalized with the thermal flame thickness of the reference laminar flame. It should be noted that the data are sampled at the reaction zone layer, i.e., c = 0.8. The results show that the local equivalence ratio is positively correlated with the flame front curvature. Furthermore, increasing the Karlovitz number results in the joint PDF becoming wider. To unlock the underlying mechanism behind the positive correlation between the local equivalence ratio and the flame front curvature, it is required to investigate the molecular diffusion terms in the species transport equation. The total molecular diffusion flux (MD_T) could be written as follows [54, 5, 50, 28]:

$$MD_{\rm T} = n_m \cdot \nabla(\rho D_m n_m \cdot \nabla Y_m) - \rho D_m |\nabla Y_m| \nabla \cdot n_m + \nabla \cdot (\rho D_m \frac{Y_m}{MW} \nabla MW),$$
(4)

where D_m is the diffusivity of species m evaluated by $D_m = (1 - Y_m) \left(\sum_{j \neq m} X_j / D_{mj} \right)^{-1}$, where Y_m is the mass fraction of species m, and D_{mj} is the binary diffusion coefficient between two species m and j. Here n_m is the unit vector normal to an iso-surface evaluated as $n_m = -\nabla Y_m / |\nabla Y_m|$, and MW is the molecular weight of the mixture. The first (second) term on the R.H.S. of Eq. 4 is the normal diffusion (curvature) term, and the last term corresponds to the molecular diffusion flux due to the gradient of the molecular weight of the mixture. It should be emphasized that the last term on the R.H.S. of Eq. 4 is fairly negligible. Therefore, it is excluded from further analysis in this study. The diffusion flux terms for the molecular hydrogen against the flame front curvature are shown in Figs. 11(a) and 11(c) for cases L and M, respectively. The diffusion fluxes have been normalized with the total diffusion flux values of

the reference laminar flame, and the flame front curvature has been normalized with the laminar thermal flame thickness. The results show that for the molecular hydrogen, the curvature and total diffusion flux terms are positively correlated with the flame front curvature, and the normal diffusion term does not have any correlation with the flame front curvature. This indicates that the molecular hydrogen diffuses strongly into the positively curved zones from the reactants. It should be noted that the positive correlation between the total diffusion flux term of molecular hydrogen with the flame front curvature could result in having higher molecular hydrogen concentration on positively curved regions (not shown for brevity). This could then explain the trend observed in Fig. 10(c-d). In addition, the curvature and total diffusion flux terms are negatively correlated with the flame front curvature for the atomic hydrogen, while the normal diffusion flux term is not dependent on the flame front curvature (Figs. 11(b) and 11(d)). This shows the enhanced diffusion of the atomic hydrogen to the unburned zone when the flame front is concave towards the reactants. A similar trend was observed very recently by Lee et al. [28] and Rieth et al. [29] for lean premixed turbulent hydrogen/air flames (located within the thin reaction zones regime) and preheated ammonia/hydrogen/nitrogen/air flames (located within the broken reaction zone regime), respectively.

It should be noted that the production rates of molecular hydrogen and ammonia with respect to the flame front curvature are shown in Fig. 12 for both turbulent test cases. The production rates have been normalized with the corresponding values obtained from the reference laminar flame, and the laminar thermal flame thickness has been utilized to normalize the flame front curvature. The negative (positive) sign of the net production rate implies that the species is consumed



Figure 10: Local equivalence ratio with respect to the progress variable for (a) case L, and (b) case M. The scatter data and the solid lines are for the turbulent cases, and the dashed lines are for the laminar case. Joint PDF of the local equivalence ratio with respect to the normalized flame front curvature for (c) case L, and (d) case M. The data are conditioned at c = 0.8, and the flame front curvature has been normalized by the laminar thermal flame thickness.

(produced). The results show a negative correlation of hydrogen production rate with the flame front curvature for both cases, and the absolute values of production rate are higher in positively curved regions compared to the corresponding values in negatively curved zones. Therefore, the hydrogen consumption rate is enhanced in positively curved regions. However, the net production rate of ammonia is not strongly dependent on the flame front curvature. It could be concluded



Figure 11: Diffusion flux terms for the molecular hydrogen for (a) case L, and (c) case M, and diffusion flux terms for the atomic hydrogen for (b) case L, and (d) case M with respect to the normalized flame front curvature. The fluxes have been normalized by the corresponding values obtained from the reference laminar flame, and the flame front curvature has been normalized by the laminar thermal flame thickness. The normal, curvature, and total diffusion terms are denoted as MD_1 , MD_2 , and MD_T . The data are conditioned at c = 0.8.

from Figs. 10-12 that the preferential diffusion of molecular hydrogen results in enhanced fuel consumption rate and local equivalence ratio on positively curved regions for the test cases studied herein. This observation is in line with previous studies showing the enhanced burning rate/fuel consumption rate based on

2-D/3-D DNS using simple/detailed chemistry, see, e.g., Rutland and Trouvé [23], Haworth and Poinsot [24], Day et al. [26], Aspden [27], Lee et al. [28], and Rieth et al. [29].



Figure 12: Production rates of hydrogen and ammonia for (a)-(b) case L, and (c)-(d) case M with respect to the normalized flame front curvature, respectively. The production rates have been normalized by the corresponding values obtained from the reference laminar flame, and the flame front curvature has been normalized by the thermal flame thickness. The data are conditioned at c = 0.8.

4. Concluding remarks

The open-source CFD toolbox OpenFOAM was utilized to perform quasi-DNS for stoichiometric planar turbulent NH₃/H₂/air flames with detailed chemistry and the mixture-averaged transport model. The blending ratio indicating the amount of hydrogen concentration in the ammonia/hydrogen mixture was equal to 0.4. The reactants temperature and pressure were set to 298 K and 1 atm, respectively. The initial non-dimensional turbulence intensity was varied from 4 to 10, and the non-dimensional integral length scale was fixed to 3.5. Therefore, the turbulent Karlovitz number was varied from 4.28 to 16.90. The chemical kinetic mechanism developed by Stagni et al. [37] consisting of 31 species and 203 reactions was used, and the recently developed open-source dynamic load balancing model (DLBFoam) was utilized to overcome the computational load imbalance among processors. The main findings for the current work are summarized as follows:

1. Under the turbulent conditions, the conditional mean profiles of NH_3 and H_2O were relatively identical to their counterpart profiles of the reference laminar flame, while the conditional mean profiles of H_2 and H deviated from their reference laminar flame due to the turbulent mixing and preferential diffusion.

2. The averaged value of the density-weighted flame displacement speed was higher than the unstrained premixed laminar burning velocity across the flame brush. Therefore, the flame elements, on average, propagated faster than the unstrained premixed laminar flame. Furthermore, the density-weighted flame displacement speed was shown to be negatively correlated with the flame front curvature.

3. The turbulent burning velocity and the wrinkled flame surface area increased by about 35% with increasing the Karlovitz number from 4.28 to 16.90. In addition, the mean flame stretch factor was higher than unity for both turbulent cases indicating the flamelet consumption velocity, on average, was higher than the unstrained premixed laminar burning velocity.

4. The mean value of the local equivalence ratio across the flame brush under turbulent conditions deviated from its laminar counterpart. Furthermore, the local equivalence ratio was shown to be positively correlated with the flame front curvature, and this observation could be attributed to the preferential diffusion of hydrogen.

5. The diffusion flux of molecular hydrogen was positively correlated with the flame front curvature indicating the enhanced diffusion of molecular hydrogen from the reactants into the positively curved zones. Furthermore, the diffusion flux of atomic hydrogen was shown to be negatively correlated with the flame front curvature, and it was shown to be intensified towards the unburned region in negatively curved regions.

6. The net production rate of the molecular hydrogen was strongly dependent on the flame front curvature, and the absolute value of the net production rate of hydrogen was higher in positively curved regions than in negatively curved zones. This could be reflected as the enhanced burning rate in positively curved regions.

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