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A comparative analysis of plasma and hydrogen effects on premixed ammonia combustion

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ABSTRACT

In this study, we use direct numerical simulations to investigate turbulent premixed ammonia flames assisted by non-equilibrium nanosecond plasma discharges and hydrogen addition. The results reveal the coupling effects of turbulence, the hydrogen concentration in the fuel blend, and plasma discharges on the microscopic structure of the flame and chemical pathways. It is found that the flame front assisted by plasma is more distributed, whilst 58 % less stretched when compared to the hydrogen-enriched un-assisted flame. Additionally, turbulence has more pronounced effects on the hydrogen-enriched flame, broadening the flame brush. A comparison of the reaction pathways contributing to the heat release indicates that turbulence shifts the key reactions producing heat from HNO+ $H \approx$ NO+ H_2 and OH+ $H_2 \approx H + H_2$ O to NH₂ dissociation reactions. Additionally, NOx emissions are more influenced by thermal effects in the hydrogen-enriched flame, with NO concentration being 35 % higher than in the plasma-assisted flame. The higher NOx emissions in the hydrogen-enriched flame are attributed to the higher concentration of H radicals, which react with HNO and produce NO.

1. Introduction

Ammonia is considered the low-hanging fruit in industrial decarbonisation, considering the relatively high production and transportation costs of other carbon-free fuels [1]. However, the primary challenge in using ammonia in conventional engines is its lower reactivity than typical hydrocarbon fuels [2]. There are several strategies to enhance the reactivity of ammonia. Blending ammonia with reactive carbon-free fuels, such as hydrogen, is known to be one of the most effective methods [3-8]. However, this approach substantially increases NOx emissions by raising the concentration of OH radicals under lean conditions [6,8,9]. Preheating the fresh mixture is another strategy to increase ammonia reactivity [10]. However, this method is only effective if the mixture temperature is increased substantially [11]. An alternative approach to assist combustion includes plasma discharges. Plasma discharges boost fuel dissociation and radical pool formations while raising the mixture temperature [12-16]. The thermal effects of plasma are less pronounced in non-equilibrium discharges than in equilibrium thermal plasma pulses [15].

It has been recently shown that nonequilibrium nanosecond plasma discharges, NSD, can effectively assist ammonia flames [17,18]. Zero and one-dimensional numerical analyses have revealed that plasma discharges can significantly shorten the ignition delay time of ammonia mixtures by up to \sim 85 % [19–23], increase the extinction strain rate of ammonia flames [8], and raise the flame speed of NH₃/O₂/He, NH₃/O₂/N₂ and NH₃/H₂/O₂/N₂ mixtures [8,20]. These investigations have shown that the number of pulses, initial mixture properties, plasma repetition frequency, reduced electric field, and pulse energy densities are the key parameters in controlling plasma-assisted ammonia combustion [19-21]. Previous studies also revealed that high-energy plasma discharges can activate the DeNOx mechanism to lower NOx emissions of lean ammonia flames [8,17,20] while broadening the preheating zone of the flames by generating radical pools [8,20]. Recent experimental studies have demonstrated that NOx formation is controlled by electron-impact reactions and collisional quenching of excited species during plasma discharges [24]. We have recently employed direct

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numerical simulations, DNS, to compare the effects of plasma and preheating on ammonia/air flames [25]. The results showed that plasma is more effective than preheating in assisting ammonia flames, especially under lean conditions [25]. Furthermore, it was demonstrated that, compared to preheated flames, plasma-assisted cases are less affected by turbulence, while they produce noticeably lower NOx emissions [25].

In our previous investigations, we compared the impacts of plasma and hydrogen on ammonia/air combustion by performing zero and onedimensional simulations, excluding the turbulence effects [25]. In this study, we aim to investigate these strategies under a turbulent condition and quantify their isolated and coupled impacts on the microscopic structure of ammonia flames using DNS. This paper is structured as follows: Section 2 introduces the numerical method and setup, the results are presented in Section 3, followed by the conclusions in Section 4.

2. Numerical method and setup

2.1. Numerical method

Direct numerical simulations were performed using a code developed in the OpenFOAM platform [26]. This code, solving equations for the conservation of mass, momentum, energy, and species, has been extensively validated and utilised in the past for different mixtures, namely NH₃/CH₄/air, n-heptane/air, and ethanol/air [25,27–32]. Previous studies have successfully employed OpenFOAM for DNS of turbulent combustion under conditions similar to this work [33–37]. To further validate the code, we have simulated a one-dimensional freely propagating laminar NH₃/air flame. The results are compared with those obtained with Cantera [38] and are presented in the supplementary materials (Section S1). To maintain the turbulent flow non-decaying, we implemented the method proposed by Bassenne et al. [39], in which a source term is introduced into the momentum equation, as outlined below,

$$\begin{aligned} \frac{\partial \rho \, \overrightarrow{v}}{\partial t} + \nabla \cdot (\rho \, \overrightarrow{v} \, \overrightarrow{v}) &= -\nabla p + \nabla \cdot \mu \left(\nabla \, \overrightarrow{v} + (\nabla \, \overrightarrow{v})^T - \frac{2}{3} I \nabla \, \overrightarrow{v} \right) \\ &+ \rho \, \frac{\varepsilon - G[k - k_{\infty}]/t_{l,\infty}}{2k} \left(\overrightarrow{v} - \overrightarrow{v}_{Ave} \right), \end{aligned} \tag{1}$$

where $\vec{\nu}$ is the velocity, ρ is the density, p is the pressure, μ is the viscosity, and the last term on the right-hand side serves as the forcing term to sustain the non-decaying turbulence. In this term, ε is the turbulent dissipation, k is the turbulent kinetic energy, k_{∞} is the turbulent kinetic energy at the initial condition, $\vec{\nu}_{Ave}$ is the averaged value of the velocity, and $t_{l,\infty}/G$ is the time constant, which is on the order of the numerical time step size.

Here, transport properties, e.g., diffusion coefficients, were determined by fitting polynomials to the NIST database for the range of the operating conditions considered in this paper [32]. Additionally, we used the semi-empirical Wilke formula to compute viscosity [40]. Differential diffusion effects were considered to determine the thermal conductivity. Furthermore, Ludwig-Soret effects were included to calculate the diffusion velocity. The ammonia combustion was modelled using the mechanism proposed by Han et al. [41], while plasma kinetics were modelled by utilising our previously developed mechanism for NH₃/H₂/O₂/N₂/He mixtures [8]. The cross-section data necessary for plasma kinetics modelling were obtained from the LXCat database [42].

In this study, temporal terms were discretised using a second-order implicit method, and a second-order central difference scheme was employed to discretise spatial terms. Additionally, fourth-order schemes were used for interpolation.

2.2. Assumptions and limitations

In the plasma-assisted cases, we used a scale separation assumption,

considering the significant differences between the time scales of electron-impact reactions (typically on the order of nanoseconds) and those associated with the smallest flow scale structures. The proposed two-stage computational strategy provides a significant speedup, effectively enabling DNS of plasma-assisted turbulent combustion with detailed chemistry, a task previously deemed impossible due to computational constraints. In this way, the unburned gas mixture is initially stimulated with a series of nanosecond discharges, modelled as square-shaped waves, within a constant volume reactor by coupling ZDPlaskin [43] with Cantera [38] codes. Then, the properties of the resulting stimulated mixture, including the mass fraction of species and temperature, are used to initialise the DNS calculations, as shown in Fig. 1b We have thoroughly validated this approach in our previous studies [8,20]. Further validation is provided here by comparing the results from two computational scenarios: one with plasma scale separation assumptions ("Separated") and one without ("Coupled"). In the Separated approach, each time step is split into calculations of the Boltzmann equations using ZDPlaskin, followed by the integration of thermal reactions ODEs, whereas in the coupled approach, both plasma and thermal kinetics are solved simultaneously. As shown in Fig. R3 in the supplementary materials (Section S2), the discrepancies between the two scenarios are negligible, showing the validity of the plasma scale separation assumption.

However, one can arguably envisage seniors wherein the abovementioned assumption potentially excludes some of the features of plasma-assisted combustion, namely the interplay between consecutive plasma discharge kernels and the acoustic waves emitted during the discharges, which could affect the localised effects of plasma on combustion. Unfortunately, accounting for such effects would significantly increase the computational costs, given the order of magnitude differences between the time scales of plasma and thermal reactions and the number of transport equations for chemical species. Therefore, we choose to focus our investigation on the conditions in which the plasmaproduced radicals are uniformly distributed upstream of the flame, similar to that in the coaxial electrode configuration in low swirl burners [44-46], as schematically shown in Fig. 1(a). This is a proven, highly effective setting for gas turbine applications [47] and is the primary focus of the current study. Given the turbulent condition considered here, it is expected that the partially oxidised ammonia and plasma radicals are sufficiently mixed within the plasma coaxial tube and over the flame lift-off length, forming a homogenous mixture of plasma-generated radicals, ions and partially oxidised fuel upstream of the flame front. Further investigations are required to determine the localised effects of plasma on combustion.

2.3. Numerical setup

Fig. 1(b) shows the three-dimensional computational domain with dimensions of $9\delta_0 \times 4.5\delta_0 \times 4.5\delta_0$ in the x, y, and z directions, respectively. Here, δ_0 represents the laminar flame thickness of an unassisted ammonia flame propagating into reactants with an equivalence ratio of 0.8, a temperature of 300 K, and a pressure of 1 atm [25]. We used this equivalence ratio to demonstrate the impact of NSD on the production/mitigation of NO, as it is well known that at \sim 0.8–0.9, such an emission attains its peak in ammonia-air premixed flames [2]. The dimensions of the computational domain are within the range of those used in the previous DNS studies [48,49]. In this study, we applied periodic boundary conditions to all boundaries, consistent with flame propagation in a constant volume reactor. We used the Passot-Pouquet method [50] to introduce turbulence at the initial condition with a velocity fluctuation of 5.5 m/s and an integral length scale ranging from 0.3 to 1.7 mm. The selected turbulent fluctuation level falls within the range prevailing in internal combustion engines [51] and matches those used in previous experimental studies on turbulent premixed NH₃/air flames [52]. With these settings, the computational domain size in each direction is at least 5 times the integral length scale.



Fig. 1. (a) Schematic of a nanosecond plasma system with the coaxial distribution of electrodes assisting a freely propagating flame and (b) computational domain and flame fronts coloured by heat release rate.

Initially, the domain was filled with burned gases at the centre and fresh mixture on the sides, a configuration also used in our previous studies on flame propagation in H₂/air and preheated and plasmaassisted NH₃/air mixtures [25,53]. The unburned gases were initially at 300 K and 1 atm with an equivalence ratio of 0.8. We obtained the composition and thermodynamic conditions of the burned gases by performing one-dimensional simulations of freely propagating laminar NH₃/air using the same initial thermodynamic conditions, results in the propagation of two flame fronts toward the x-direction, as illustrated in Fig. 1(b). In this figure, the flame front is discerned by plotting the isosurface of the progress variable at which the heat release reaches its maximum value, c^* . In this study, the progress variable is defined as follows,

$$c = \frac{Y_{H_2O}}{Y_{H_2O,eq}} \tag{2}$$

where Y_{H_2O} and $Y_{H_2O,eq}$ are the mass fractions of the H₂O molecule and its corresponding value at the equilibrium condition, respectively.

Table 1 presents the details of the simulated cases, including the hydrogen mole fraction in the fuel, X_{H2} , equivalence ratio, φ , fresh mixture temperature, T_{in} , number of nanosecond discharges, N_{NSD} , laminar flame speed, S_L , laminar flame thickness, δ_L , Kolmogorov length scale, η , Karlovitz number, Ka, and Damköhler number, Da. Furthermore, the selected cases are shown in the Peters-Borghi diagram in the supplementary materials (Section S3 – Fig. R4). To comparatively assess the effects of hydrogen content in the mixture and plasma discharges on ammonia combustion, three fuel compositions were considered, namely 0.43NH₃/0.57H₂, NH₃ assisted by NSD (NH₃/NSD), and 0.72NH₃/

Table 1

Key parameters of the investigated cases; X_{H2} is the hydrogen mole fraction in the fuel, φ is the equivalence ratio, T_{in} is the initial mixture temperature, n is the number of nanosecond plasma discharges, S_L is the laminar flame speed, δ_L is the laminar flame thickness, η is the Kolmogorov length scale, Ka is the Karlovitz number, and Da is the Damköhler number.

Properties	$\rm NH_3/\rm NSD$	$0.43 \text{NH}_3 / 0.57 \text{H}_2$	0.72NH3/0.28H2/NSD
X _{H2} [%]	0	57	28
Φ	0.8	0.8	0.8
T_{in} [K]	300	300	300
N _{NSD}	100	0	58
$S_L [\rm cm/s]$	34.2	34.2	34.2
δ_L [mm]	1.1	0.52	0.82
η [mm]	0.225	0.107	0.167
Ка	23.8	23.8	23.8
Da	0.456	0.456	0.456

0.28H2 assisted by NSD (0.72NH3/0.28H2/NSD) reacting with air as the oxidiser. To ensure comparability, the number of plasma discharges and hydrogen content of 0.43NH₃/0.57H₂ and 0.72NH₃/0.28H₂/NSD mixtures were selected to match their laminar flame speeds to that of the NH₃/NSD flame, in which the flame was assisted by 100 nanosecond plasma pulses. Under this assumption and as shown in Fig. 2, the $0.72NH_3/0.28H_2/NSD$ flame was stimulated by 58 plasma pulses to match its laminar flame speed with that of the NH₃/NSD flame assisted by 100 pulses. In plasma-assisted cases, the pulse repetition frequency, PRF, was 50 kHz, the reduced electric field, E/N, was 350 Td, and the pulse energy density, E_p , was 5 mJ/cm³. The plasma regime and its settings were selected based on commonly used plasma generators [54, 55] and our previous studies on plasma-assisted NH₃/air and $NH_3/H_2/air$ combustion [8,20]. Here, the specified E_p was achieved by adjusting the pulse width. Our previous studies showed that resolving the pulse width with at least 2000 time steps is enough to achieve resolution-independent results in plasma-assisted combustion [8,20]. Considering this, we used 3000 time steps to capture plasma reactions during each discharge. Details of the utilised initial condition for the plasma and CFD simulations are presented in Table R1 in the supplementary materials (Section S4).

The computational domain was meshed using Cartesian grids, with $600 \times 300 \times 300$ cells in the x, y, and z directions, respectively. The thermal flame thickness was captured with 16 grids while resolving the Kolmogorov length scale. This grid resolution is consistent with those



Fig. 2. Laminar flame speed as a function of the number of plasma discharges in NH₃/NSD and 0.72NH₃/0.28H₂/NSD cases.

used in the literature for DNS of premixed flames [5,56–59]. Additionally, we selected the temporal resolution of the DNS to ensure that Courant-Friedrichs-Lewy, CFL, always remained below 0.1.

3. Results and discussions

Fig. 3 shows the conditional mean of heat release rate, $\langle HRR \rangle$, as a function of the progress variable defined in Eq. (2). In turbulent cases, (*HRR*) is calculated by determining the mean value of the heat release in computational cells that were categorised based on the progress variable value, which was divided into 100 equal intervals between 0 and 1. The selected mixtures were also simulated under laminar conditions using Cantera, and the results are depicted in Fig. 3. The results show that raising the contribution of H₂ in assisting the flame leads to a substantial increase in the heat release rate while shifting the maximum heat release rate toward lower progress variables. Furthermore, as anticipated, introducing H₂ to the fuel substantially activates the flame preheat zone. Comparing laminar and turbulent cases shows that the flame's response to turbulence depends on the hydrogen content in the fuel. Turbulence lowers the $\langle HRR \rangle$ across all progress variable values, both for NH₃/NSD and 0.72NH₃/0.28H₂/NSD flames, while it significantly amplifies it for 0.43NH₃/0.57H₂ flame. We extensively studied the NH₃/NSD flame in our recent publication [25]. Therefore, here, we mainly focus on the distinctive characteristics of the 0.43NH₃/0.57H₂ and 0.72NH₃/0.28H₂/NSD flames.

3.1. Microscopic flame features

Further comparisons of the impacts of hydrogen and plasma are elucidated in Fig. 4, showing spatial distributions of the heat release rate, mass fraction of HO₂, local elemental equivalence ratio, and mass fraction of H. Here, the flame front is delineated by the isoline of $c=c^*$, shown by white lines in Fig. 4. Here, the elemental equivalence ratio is defined as below,

$$\phi_e = \frac{\left(\frac{J_H}{J_O}\right)}{\left(\frac{J_H}{J_O}\right)_{st}},\tag{3}$$

where J_H is the elemental mass fraction of the H atom, J_O is the elemental mass fraction of the O atom, and subscript "*st*" indicates values under the stoichiometric condition. The elemental mass fractions are calculated using,



$$J_i = \sum_{j=1}^{N} \frac{W_i}{W_j} \alpha_{ij} Y_j, \tag{4}$$

where W_i is the atomic weight of the element *i*, W_j is the molecular weight of the species *j*, α_{ij} represents the number of atoms of type *i* in species *j*, Y_j is the mass fraction of species *j*, and *N* is the total number of species [60].

Fig. 4(I) shows that the 0.43NH₃/0.57H₂ flame is highly wrinkled and relatively thin, except where it is intensely strained by turbulent structures. Conversely, the 0.72NH₃/0.28H₂/NSD flame, despite falling within the thin flame regime according to the Borghi diagram, appears more distributed. This is further supported by Fig. 4(II), showing that the HO₂ radical is noticeably more distributed upstream of the plasmaassisted flame than the 0.43NH₃/0.57H₂ flame. To quantify these differences, the mean value of conditional curvature at $c=c^*$, denoted as $\langle \kappa^* \rangle$, is calculated for the investigated flames using

$$\kappa = \nabla \cdot \overrightarrow{n},\tag{5}$$

where \overrightarrow{n} is the flame normal vector defined as below,

$$n = -\frac{\nabla c}{|\nabla c|}.$$
(6)

The analyses show that $\langle \kappa^* \rangle$ is 389 and 165 [m⁻¹] in 0.43NH₃/0.57H₂ and 0.72NH₃/0.28H₂/NSD flames, respectively. To quantify the effects of turbulence on the flames, the conditional mean of the surface density function, $|\nabla c|$, is calculated and plotted against the progress variable in Fig. 5(a). This quantity is inversely proportional to the flame thickness, which is non-dimensionalised by multiplying it by the laminar flame thickness [61]. The turbulent cases are colour-coded by the conditional mean value of the elemental equivalence ratio.

As shown in Fig. 5(a), the 0.43NH₃/0.57H₂ flame is more susceptible to flame thinning as a result of turbulent stretching than the 0.72NH₃/ 0.28H₂/NSD flame. This is further demonstrated in Fig. 5(b) by plotting the spatial distribution of the magnitude of the temperature gradient along with the isolines of the progress variable at c = 0.5, 0.7, and 0.9,coloured by temperature. The results show that the temperature gradient is significantly higher upstream of the 0.43NH₃/0.57H₂ turbulent flame than the $0.72NH_3/0.28H_2/NSD$ flame, leading to a thinner flame. Fig. 5(a) further reveals that the thinning of the $0.43NH_3/0.57H_2$ turbulent flame is accompanied by a reduction in the elemental equivalence ratio, e.g., at c = 0.5, indicating that the thinning is not due to the preferential diffusion. Interestingly, unlike the hydrogen-enriched case, turbulence has a limited impact on the flame thickness in the plasmaassisted flame. Here, the flame surface area under the turbulent condition, A_T , is determined by integrating the surface density function over the volume, V, across the computational domain.

$$A_T = \int |\nabla c| dV. \tag{7}$$

In Eq. (7), A_T is non-dimensionalised by the domain cross-section, A^0 , which is $4.5\delta_0 \times 4.5\delta_0$. It is found that A_T/A^0 is 5.07 for the 0.43NH₃/ 0.57H₂ flame, whereas it is 3.52 for the turbulent 0.72NH₃/0.28H₂/NSD flame.

Fig. 4 (III) also shows that the elemental equivalence ratio, ϕ_e , undergoes more pronounced changes near the 0.43NH₃/0.57H₂ flame compared to the plasma-assisted flame, which is particularly notable in the post-flame zone. This reflects the higher preferential diffusion of H radicals in 0.43NH₃/0.57H₂ flame, as illustrated in Fig. 4(IV). The concentration of H radicals is higher in the convex parts of the flame (where κ > 0) compared to the concave parts (where κ < 0), which aligns with previous numerical findings by Netzer et al. [62] on laminar NH₃/H₂/air flames. This observation is further supported by Fig. 6, which shows the conditional mean of the mass fraction of H as a function of curvature at *c*=*c**. The conditional mean of the mass fraction of



Fig. 4. Spatial distributions of (I) heat release rate, (II) mass fraction of HO₂, (III) local elemental equivalence ratio, and (IV) mass fraction of H. The white line shows the flame front using $c=c^*$.



Fig. 5. (a) Conditional mean of the surface density function as a function of progress variable and (b) spatial distribution of temperature gradient with isolines of c = 0.5, 0.7, 0.9 isolines coloured with temperature.



Fig. 6. Conditional mean of mass fraction of H as a function of curvature at $c{=}c^{\ast}.$

hydrogen atoms increases almost linearly with curvature in both cases. Additionally, the results indicate that the conditional mean of Y_H is six times higher in the 0.43NH₃/0.57H₂ flame compared to the plasma-assisted flame.

Analysing the cross-correlation between the heat release and elemental equivalence ratio conditioned on the progress variable shows that these quantities are weakly correlated, specifically in the $0.43NH_3/0.57H_2$ flame, where the cross-correlation factor is smaller than 0.1. Fig. 7 shows the conditional temperature as a function of the progress variable in laminar and turbulent cases. Here, the values of $c=c^*$ are indicated by vertical black and red dash-dot lines for turbulent $0.43NH_3/0.57H_2$ and $0.72NH_3/0.28H_2/NSD$ flames, respectively. It can be found that introducing turbulence results in an almost identical drop in the temperature at the flame front. These results reveal that the spatial variations of the elemental equivalence ratio and thermal effects have limited direct impacts on the heat release rate in turbulent $0.43NH_3/0.57H_2$ and $0.72NH_3/0.28H_2/NSD$ flames. Considering these findings, the main distinct features of the selected flames were further evaluated by focusing on the key chemical pathways contributing to heat release in



Fig. 7. Conditional mean of temperature as a function of progress variable.

Section 3.2.

3.2. Reaction pathways

Key reactions driving heat release and its consumption in the selected laminar and turbulent flames are outlined in Fig. 8 as a function of the progress variable. The selected reactions contribute at least 5 % to the heat release or consumption. The corresponding contributions of these reactions at the flame front, i.e., at $c=c^*$, are summarised in Fig. 9. The results reveal that turbulence significantly reduces the contributions of HNO+ $H \Rightarrow$ NO+ H_2 , OH+ $H_2 \Rightarrow H + H_2$ O, and NH+NO \Rightarrow N₂O+H reactions in the heat release while increasing the heat produced by NH₂+OH \Rightarrow NH+H₂O reaction. Fig. 8 shows that the key reaction releasing heat upstream of the laminar flames is NH₂+NO \Rightarrow N₂+H₂O. Interestingly, unlike in the 0.72NH₃/0.28H₂/NSD flame, turbulence changes the source of the heat release upstream of the 0.43NH₃/0.57H₂ flame by diminishing the impact of NH₂+NO \Rightarrow N₂+H₂O and amplifying the contribution of $H + O_2 \Rightarrow HO_2$. The activation of the $H + O_2 \Rightarrow HO_2$ reaction in the turbulent 0.43NH₃/0.57H₂ flame explains why the



Fig. 9. Main reactions contributing to heat production and consumption in laminar and turbulent $0.43NH_3/0.57H_2$ and $0.72NH_3/0.28H_2/NSD$ flames at $c=c^*$.

concentration of HO₂ is significantly higher in this flame compared to the 0.72NH₃/0.28H₂/NSD flame, as shown in Fig. 4(II). This highlights that the key radical indicator of the reactivity of the preheating zone is highly dependent on both turbulence and mixture composition. Figs. 8 and 9 also reveal that $H + O_2 \simeq O + OH$ is the main sink for heat for all the studied flames. However, $2OH \simeq O + H_2O$ consumes more heat in $0.72NH_3/0.28H_2/NSD$ flame than in $0.43NH_3/0.57H_2$ flame.

The following part of the paper aims to assess the effects of hydrogen and plasma on NO formation, a critical challenge in ammonia combustion. Fig. 10(I) shows spatial distributions of NO in the studied cases, revealing significantly higher NO levels in the $0.43NH_3/0.57H_2$ flame compared to the $0.72NH_3/0.28H_2/NSD$ flame. Calculations indicate that the volume integration of NO in the $0.43NH_3/0.57H_2$ flame is 35 % higher than that in the $0.72NH_3/0.28H_2/NSD$ flame.

Fig. 11 shows NO pathways in $0.43NH_3/0.57H_2$ and $0.72NH_3/0.28H_2/NSD$ flames. The results show that, in both cases, the primary contributor to NO production is the HNO+ $H \Leftrightarrow H_2$ +NO reaction. The higher preferential diffusion of H radicals in $0.43NH_3/0.57H_2$ flame



Fig. 8. Main reactions contributing to heat production and consumption in laminar and turbulent 0.43NH₃/0.57H₂ and 0.72NH₃/0.28H₂/NSD flames.



Fig. 10. Spatial distributions of (I) mass fraction of NO and (II) production/consumption rate of NO The white line shows the flame front using $c=c^*$.



Fig. 11. Path flux of NO in $0.43 \rm NH_3/0.57 \rm H_2$ (black) and $0.72 \rm NH_3/0.28 \rm H_2/NSD$ (red) flames.

raises the concentration of H radicals near the flame, leading to more pronounced NO generation, compared to $0.72NH_3/0.28H_2/NSD$ flame, through the reaction with HNO. This explains why NO emission is higher in $0.43NH_3/0.57H_2$ flame than in $0.72NH_3/0.28H_2/NSD$. This correlation is further supported by comparing spatial distributions of the mass fraction of H (Fig. 4(IV)) and the rate of NO production/consumption, $\dot{\omega}_{NO}$, (Fig. 10(II)). The relatively lower concentration of H radicals in the plasma-assisted flame activates the HNO(+*M*) \approx *H*+NO(+*M*) third body reaction, an inactive reaction in the 0.43NH_3/0.57H_2 flame. Fig. 11 also indicates that, in both cases, NO is mainly consumed by NH and NH₂.

Fig. 12 shows the dependency of the NO production/consumption rate as a function of the heat release rate. Results reveal a distinct



Fig. 12. Dependency of the conditional mean of NO production/consumption on the heat release rate.

pattern: unlike the 0.43NH₃/0.57H₂ flame, NO production in plasmaassisted flame is minimally due to the thermal effects. To further confirm this observation, the cross-correlation between the production/ consumption rate of NO and heat release rate is examined and shows a cross-correlation constant of 0.68 for 0.43NH₃/0.57H₂ flame and 0.03 for 0.72NH₃/0.28H₂/NSD flame.

4. Conclusions

Direct numerical simulations were performed to comparatively study the effects of nanosecond plasma discharges and hydrogen concentration in the fuel blend in lean premixed ammonia flames in a nondecaying turbulent flow. Results revealed that enriching the mixture with hydrogen amplifies the impacts of turbulence on the flame structure. The investigations showed that the hydrogen-enriched flame exhibits significantly more wrinkling and a higher flame surface area under turbulence than the plasma-assisted flame. Furthermore, the plasma-assisted flame is more distributed compared to the hydrogenenriched flame. It was also shown that spatial variations of elemental equivalence ratio induced by the preferential diffusion and H radical concentration are higher in the hydrogen-enriched flame. The higher concentration of H radical also results in higher NO emissions in the hydrogen-enriched flame than in the plasma-assisted case. Moreover, the NOx emissions in the hydrogen-enriched flame depend more on the thermal effects. The results also highlighted that turbulence considerably raises the contribution of NH₂ dissociation reactions in producing heat.

Novelty and significance statement

This work presents, for the first time, comparative analyses of the effects of plasma and hydrogen on ammonia/air flames under a nondecaying turbulent condition by employing direct numerical simulations and detailed plasma and thermal kinetics. The obtained results expand the current understanding of the distinct impacts of plasma and hydrogen on turbulent ammonia/air combustion, including the reaction pathways and the flame's microscopic features. This study reveals that using plasma discharges is more beneficial in assisting ammonia flames than hydrogen. Furthermore, it challenges the current understanding of turbulence effects on ammonia flames, highlighting the role of turbulence-chemistry interactions on heat release rate.

CRediT authorship contribution statement

Mohammad Shahsavari: Funding acquisition, Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Investigation, Formal analysis, Conceptualization. Nilanjan Chakraborty: Writing – review & editing, Writing – original draft, Methodology. Alexander A. Konnov: Writing – review & editing, Writing – original draft. Shenghui Zhong: Validation, Software, Methodology. Agustin Valera-Medina: Writing – review & editing, Writing – original draft. Mehdi Jangi: Writing – review & editing, Writing – original draft, Methodology, Funding acquisition, Formal analysis, Conceptualization.

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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Supplementary materials

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