

# Numerical investigation on the combustion characteristics of premixed NH<sub>3</sub>-air flames using gliding arc plasma

Ziyu Wang, B. Aravind<sup>\*</sup>, Syed Mashruk, Agustin Valera-Medina

College of Physical Sciences and Engineering, Cardiff University, Wales, CF24 3AA, UK

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## ABSTRACT

In this study, a numerical model is developed to predict the combustion characteristics of gliding arc plasma (GAP) assisted ammonia (NH<sub>3</sub>)-air mixture, integrating ZDPlasKin and Chemkin. To the best of the authors' knowledge, this is the first validated model capable of accurately predicting NO emissions from GAP-assisted NH<sub>3</sub>-air combustion. Initially, three well-known plasma mechanisms are evaluated against non-reacting GAP experiments to assess their effectiveness in modelling NH<sub>3</sub>-air plasma chemistry. The most accurate mechanism is then coupled with an optimized combustion mechanism to improve NO prediction accuracy. The results indicate that NH<sub>2</sub> radical formation is enhanced by approximately 7 % at a reduced electric field of 30 Td, playing a crucial role in NO reduction. Additionally, NH<sub>2</sub> is primarily generated through two key reactions:  $O(^1D) + NH_3 \rightarrow OH + NH_2$  and  $N_2(A) + NH_3 \rightarrow NH_2 + N_2 + H$ , occurring before combustion. Furthermore, increasing plasma power significantly accelerates NO consumption by promoting the formation of excited NH<sub>3</sub> states (NH<sub>3</sub>(e<sub>1</sub>), NH<sub>3</sub>(e<sub>2</sub>)), which enhance NH<sub>2</sub> and NH radical production. Sensitivity analysis reveals that NH<sub>2</sub> exhibits a 52.1 % sensitivity to the reaction  $N(^2D) + NH_3 \rightarrow NH_2 + H + N_2$  at 90 Td, highlighting its dominant role in NO reduction.

## 1. Introduction

Ammonia (NH<sub>3</sub>) is gaining significant attention as a promising green fuel due to its carbon-free combustion, high energy density comparable to fossil fuels (22.5 MJ/kg) [1], and cost-effective storage, positioning it as a viable solution to the current energy crisis [2]. Despite these advantages, NH<sub>3</sub> has high NO<sub>x</sub> emissions due to its inherently low flame temperature, low laminar combustion rate, and low flammability [3]. To circumvent these issues, co firing of NH<sub>3</sub> with highly reactive fuels [4], such as methane [5] and hydrogen [6], staged combustion [7], humidification [8], plasma assisted combustion [9] etc. are commonly adopted techniques.

Among these techniques, plasma assisted combustion [10], is relatively new strategy and, with great potential to enhance the flame stability and other combustion characteristics [9,11]. Although its impact on NH<sub>3</sub> combustion is comparatively less explored, recent studies [12–14] have shown that plasma can significantly address the drawbacks of NH<sub>3</sub> as a future fuel [15]. However, plasma assisted combustion of NH<sub>3</sub> does not alter the primary NO generation pathway, where HNO is involved in 70 % of the reaction [16]. This suggests that a careful

analysis of the reaction pathways involved in plasma-assisted combustion of NH<sub>3</sub> is essential to understand NO<sub>x</sub> consumption through the production of NH radicals [17]. The dielectric barrier discharge (DBD) assisted NH<sub>3</sub> combustion on the premixed NH<sub>3</sub>-H<sub>2</sub>-air, revealed that NO<sub>x</sub> emissions increases with the plasma in laminar/turbulent flames [18]. While Ju et al. [14] found that NO has been reduced significantly using gliding arc plasmas (GAP), by promoting the NO consumption reactions.

In plasma assisted combustion modelling, many researchers have made a considerable contribution in DBD and nanosecond repetitively pulsed discharges (NRP) [16–22]. Faingold et al. [19] conducted a detailed parametric studies on the effect of pulse repetition frequency, number of pluses of NRP on the ignition delay time (IDT) characteristics of NH<sub>3</sub>-O<sub>2</sub>-He mixtures. Shahsavari et al. [20] investigated the impact of NRP on flame characteristics. They found that the pulse energy density increasing in the range of 0–20 mJ/cm<sup>3</sup>, at a given reduced electric field, decreases the IDT. In 2019, Mao et al. proposed a numerical model to predict the Ignition enhancement of CH<sub>4</sub>-O<sub>2</sub>-He mixtures under NRP and DC discharges [21]. Recently, Zhong et al. developed a robust kinetic model for plasma combustion of NH<sub>3</sub>-O<sub>2</sub>-N<sub>2</sub> that are validated with the experiments [22]. The same plasma mechanism was used by Mao et al.

<sup>\*</sup> Corresponding author.

E-mail address: [balakrishnana4@cardiff.ac.uk](mailto:balakrishnana4@cardiff.ac.uk) (B. Aravind).

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[23] for DBD-promoted ignition delay of  $\text{NH}_3$ -air and in the analysis of NO formation mechanisms. The IDT and NO<sub>x</sub> emission mechanisms of  $\text{NH}_3$ -air by NRP were similarly investigated by Taneja et al. [24]. Shahsavari et al. [25] constructed a specific mechanism for the action of NRP and hydrogen on the combustion of ammonia, verifying the change in temperature under specific conditions.

Although numerous experimental and numerical studies [19,20,22–27] have investigated NRP and DBD for  $\text{NH}_3$  ignition and NO formation, research on GAP for ammonia combustion has largely remained experimental [12,14,18,28]. Nevertheless, Compared with DBD and NRP, the rotating gliding arc plasma provides broad volumetric coverage and can be directly incorporated into the combustion zone, making it highly promising for enhancing combustion. Meanwhile, GAP also features a combination of high energy density and thermal effects, enabling continuous and stable discharge that effectively promotes chemical reactions in combustion. Recent studies have shown that GAP plasma combustion significantly reduces NO<sub>x</sub> emissions, drawing increasing attention from the research community [14,28,29]. However, the underlying mechanisms of NO reduction in GAP remain unclear, and existing experimental results lack comprehensive interpretation and analysis.

In this work, for the first time, numerical model is developed to study the GAP-assisted combustion characteristics of  $\text{NH}_3$ -air mixture. Initially, different plasma mechanisms are compared, the most suitable one for GAP is selected based on experimental validation. This is followed by the development of a combustion mechanism integrated with the plasma mechanism. Finally, the mechanism behind the NO emission reduction under the influence of GAP is analysed in detail.

## 2. Numerical methods and model validation

In order to validate the numerical method, GAP experiments are conducted to comprehend the effect of GAP on the  $\text{NH}_3$  conversion rate for non-reacting cases. The details of the experiment setup are shown in the [Supplementary Material Fig. S1](#). Different ratios of  $\text{NH}_3$ -air are injected from the tube, and the gas mixture is ionized by an arc formed by the high-voltage electrode. The “fresh gas” is taken above the electrode and the volume fraction of  $\text{NH}_3$  is measured using Agilent 990 microGC. The chemiluminescence spectrum of the discharge at the burner's exit and 10 cm from its central axis was recorded using a flexible AvaSpec-ULS spectrometer, where the stray light (0.19–1.0 %) represented the main source of error. This method for determining electron temperature based on the H- $\alpha$ /H- $\beta$  spectral line intensity ratio has relative errors of only  $\pm 0.017$  % [30]. Therefore, the potential overall uncertainty is estimated to below 1.017 %. The typical temporal evolution of the voltage and current waveform of GAP in the present study is shown in the [Supplementary Material Fig. S2](#). As evident from [Fig. S2](#) that voltage shows a periodic jagged shape, and current spikes are observed at each breakdown at the smallest gap. This breakdown type GAP is observed for many plasma assisted combustion studies [28]. In GAP, both spark-type discharge and glow-type discharge are observed [12]. In the present study, current reaches above 1 A and below 0.5 A are termed as spark and glow discharges.

### 2.1. Numerical method

This study adopts a numerical methodology similar to that proposed by Crispin et al. for modelling the GAP [31]. The simulation is divided into two domains, as shown in [Fig. 1](#). The first domain,  $0-t_1$ , represents the discharge length or residence time. During this period, the arc initiates at the minimum gap, peaks in current, propagates helically, elongates, and eventually breaks as the current drops to zero. The minimum clearance between the conical electrode and the tube wall is 2.5 mm, with a charging length of 14 mm from this location to the apex. This discharge time is calculated from the voltage-current curve. The second domain,  $t_1-t_2$ , is termed as the afterglow discharge. The

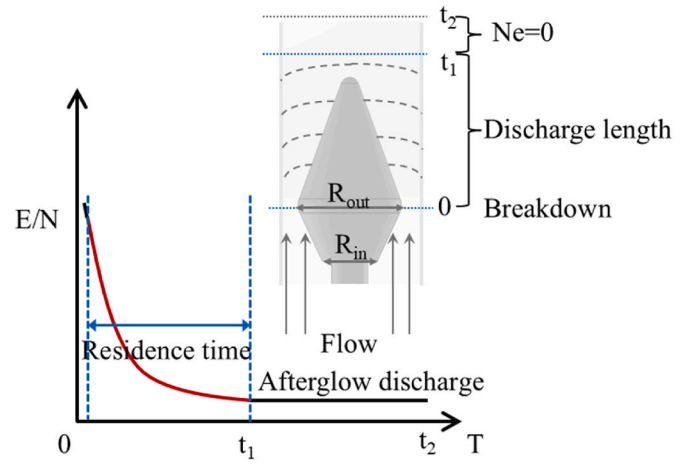


Fig. 1. Theory of gliding arc plasma.

discharge power is maintaining between 130 and 150 W, and the frequency of plasma is 11 kHz. The discharge time is between 4 and 7 ms, depends on the gas flow rate. The plasma chemistry in the afterglow region is significantly different from that of the plasma glow [23]. However, the afterglow retains most of the plasma properties.

To simplify the calculations, the reduced electric field and electron density are estimated as period averages using the voltage-current characteristic curves. This study was carried out using a dual-swirl plasma-assisted burner at CEAT, Cardiff University. Further details of this burner are available in Wang et al. [29] and Aravind et al. [32]. In the ionization region, the initial gas mixture consists of  $\text{NH}_3/\text{N}_2/\text{O}_2$ . The electron density is calculated using Eq. (1) [33]:

$$Ne = J_{av}/e\mu_e E \quad (1)$$

In Eq. (1),  $Ne$  is the current density,  $J_{av}$  is the ratio of current to cross-sectional area,  $\text{A}/\text{cm}^2$ . The electron mobility ( $\mu_e$ ) is calculated from BOLSIG+, derived from collision interface data with initial  $E/N$  intensity, divided by initial gas density,  $\text{cm}^2/\text{Vs}$ .  $E$  is electric field,  $\text{V}/\text{cm}$ .

In this study, the current curve provides the data between 0.1 and 0.11 A, the average electron conduction current density was calculated to  $1-1.16 \text{ A}/\text{m}^2$ , the electric field ( $E$ ) within the discharge region measured  $2.1 \text{ kV}/\text{cm}$ , the electron mobility ( $\mu_e$ ) is calculated at  $500 \text{ cm}^2/\text{V}$ . The electron density averaged across the conical electrode was estimated to be  $5.7 \times 10^{12} - 6.4 \times 10^{12} \text{ cm}^{-3}$ .

The  $E/N$  is determined from the experimental voltage, electrode gap length and gas density [28]. The initial gas density is estimated by initial pressure and temperature,  $2.4 \times 10^{19} \text{ cm}^{-3}$ . The voltage is estimated at 1.8–4.5 kV. In this study, the  $E/N$  is 30–90 Td. This range of reduced electric field strength is similar to that reported by Dong et al. [34].

The initial electron temperatures were preliminary determined based on spectral measurements. Spectral measurements at different mixture ratios are shown in [Fig. 2](#). The electron temperature of the plasma is estimated using Eq. (2) based on the spectral characteristics observed in experiments [30]. The electron temperature is used as an initial parameter in order to assume Maxwellian energy distribution for electrons; the value of reduced field is calculated in this case to satisfy electron energy balance. This estimation can enhance the numerical method for different  $\text{NH}_3$ -air ratios.

$$\ln(I_{32}/I_{42}) = \ln(v_{32}/v_{42}) + 1.08 + h(v_{42} - v_{32}) / (kT_e) \quad (2)$$

Where  $T_e$  is the electron temperature in Kelvin.  $I_{32}$  and  $I_{42}$  are the intensity of H- $\alpha$ (486.1 nm), H- $\beta$ (656.3 nm).  $v_{32}$  and  $v_{42}$  are frequencies of radiation initiated in nm.  $h$  is the Planck constant in J-s.  $k$  is Boltzmann constant, J/K. The system is assumed to be in local thermal equilibrium when the electron temperature of the plasma ranges between 4000 and 64,000 K. The electron temperature is used as an initial parameter in

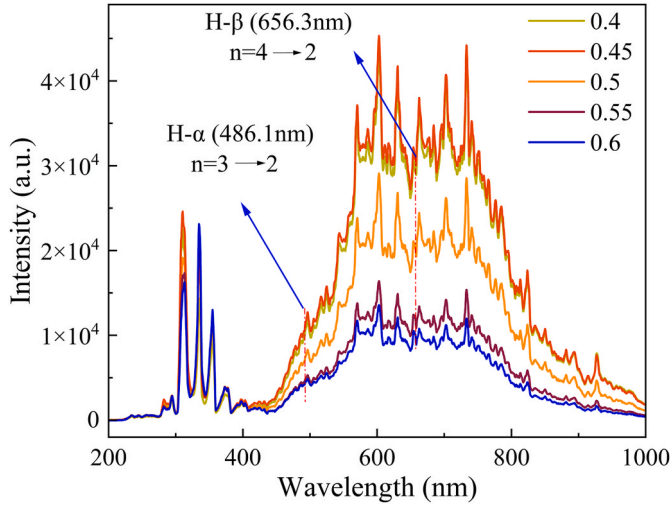


Fig. 2. Spectra of plasma at different  $\text{NH}_3$  ratios.

order to assume Maxwellian energy distribution for electrons; the value of reduced field is calculated in this case to satisfy electron energy balance.

As a transient property, the mixture density ( $\rho_{\text{mix}}$ ) dynamically adjusts to real-time composition variations, computed through the component-based formulation in Eq. (3).

$$\rho_{\text{mix}} = \frac{1}{N_A} \sum_i M_i \cdot n_i \quad (3)$$

Where  $i$  represents different species, [ $\text{NH}_3$ ,  $\text{N}_2$ ,  $\text{O}_2$  ...].  $M_i$  denotes the molar mass of species  $i$ . The number density of each component is represented by  $n_i$ .  $N_A$  is Avogadro's constant,  $6.022 \times 10^{23} \text{ mol}^{-1}$ .

The GAP reactor exhibits substantially higher gas temperatures, observed by Dong et al. [34]. Compared to conventional DBD reactors, representing a fundamental operational difference between these plasma systems. Consequently, the GAP generated thermal effects on gas mixtures should be explicitly considered in the analysis. When it taken into account, the gas temperature ( $T_{\text{gas}}$ ) can be determined through the heat transfer equation (4) under the physical condition of adiabatic equidistant approximation [35].

$$\frac{N_{\text{gas}}}{\gamma - 1} \frac{dT_{\text{gas}}}{dt} = \sum_{i=1}^{i_{\text{max}}} \pm \delta \varepsilon_i \cdot R_i + P_{\text{elast}} \cdot [N_e] + P_{\text{ex}} \quad (4)$$

$$\lambda_{\text{mix}} = \frac{1}{\rho_{\text{mix}}} \sum_i (\lambda_i \cdot C_i) \quad (5)$$

$$c_{p,\text{mix}} = \sum_i N_i \frac{\gamma_i}{\gamma_i - 1} \quad (6)$$

$$P_{\text{ex}} = \frac{N_u \cdot \lambda \cdot (T_{\text{gas}} - T_{\text{wall}})}{R_{\text{out}}^2} \quad (7)$$

$\sum_{i=1}^{i_{\text{max}}} \pm \delta \varepsilon_i \cdot R_i$  represents the heat of chemical reactions;  $P_{\text{elast}}$  corresponds to Joule heating induced by electron current, associated with elastic electron-neutral collisions (this term is computed using the BOLSIG+ solver.  $P_{\text{ex}}$  is a user-defined heat source that can be arbitrarily specified in equation (7). The symbol  $\lambda$  is used for the gas-phase thermal conductivity.  $c_p$  denotes the specific heat capacity at constant pressure.  $N_i$  and  $\gamma_i$  are the density and specific heat ratio of component  $i$ , respectively.  $C_i$  represents the concentration of the  $i$ -th gas species (where  $i$  is defined consistent with Equation (3)). The Nusselt number is fixed at  $Nu = 8$  for this analysis. The effective thermal conductivity ( $\lambda$ ) of the gas mixture is calculated as a weighted average of the constituent

species ( $\text{NH}_3$ ,  $\text{O}_2$ , and  $\text{N}_2$  ...) based on their respective concentrations. The reactor wall temperature ( $T_{\text{wall}}$ ) is held constant at the initial reaction temperature throughout the simulation. The system geometry is characterized by reactor radius  $R_{\text{out}}$ .

## 2.2. Model validation

The method of coupling ZDPlasKin [35] with Chemkin [36] has been generally validated by numerous studies, demonstrating its effectiveness in accurately simulating plasma-assisted combustion processes, including the evolution of chemical species and changes in gas temperature [22].

The plasma mechanisms of  $\text{NH}_3$ -air mixtures under plasma conditions have also been the subject of several studies [23–25]. Taneja et al. [24] assembled a reaction mechanism comprising 53 species and 383 reactions for NRP. Shahsavari et al. [25] assembled a plasma reaction mechanism comprising 61 species and 790 reactions. A plasma kinetic mechanism was constructed by integrating the  $\text{NH}_3$ - $\text{O}_2$ -He reaction mechanism proposed by Faingold et al. [19]. Mao et al. [23] provided a plasma mechanism which includes 77 species and 894 reactions. A plasma mechanism involving  $\text{NH}_3$ - $\text{O}_2$ - $\text{N}_2$  was utilized in DBD.

Although several mechanisms have been developed for NRP [24,25], no mechanism is currently available for GAP-assisted combustion of  $\text{NH}_3$ . As an initial step toward identifying the most suitable mechanism for GAP, the performance of models proposed by Mao et al. [23], Taneja et al. [24], and Shahsavari et al. [25] is compared with the present experimental results on GAP-assisted  $\text{NH}_3$  conversion in non-reacting cases. The  $\text{NH}_3$  conversion rate was calculated from the initial  $\text{NH}_3$  volume fraction and the sampled ammonia volume fraction [37].

It is evident from Fig. 3 that mechanism proposed by Mao et al. [23] demonstrates good agreement with the present experiments and is therefore selected for the subsequent simulations. Following the selection of a suitable mechanism for GAP, the plasma mechanism of Mao et al. [23] is combined then with the  $\text{NH}_3$  combustion mechanism proposed by Alnasif et al. [38,39].

During the coupling process, Alnasif's mechanism serves as the host, while Mao et al.'s mechanism functions as the donor. All plasma-related reactions from Mao's mechanism are integrated into Alnasif's mechanism, with overlapping reactions and species carefully removed. The equivalence ratio is defined as follows:

$$\Phi = \frac{(F/O)_{\text{real}}}{(F/O)_{\text{stoichiometric}}} \quad (8)$$

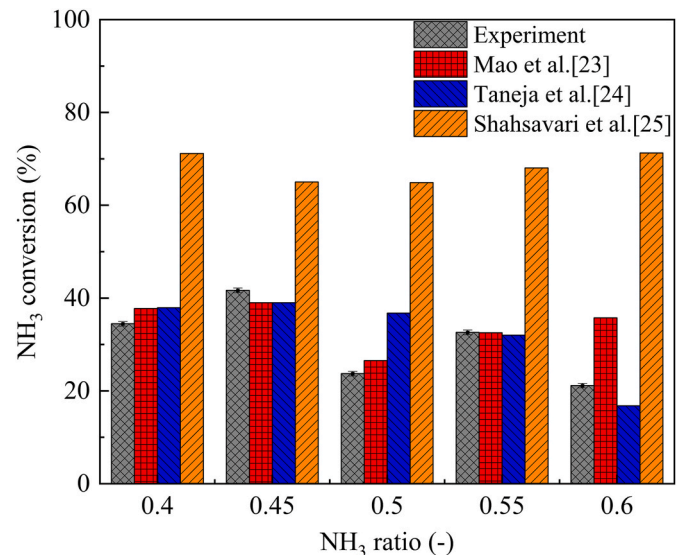


Fig. 3. Validation of  $\text{NH}_3$  plasma mechanism suitable for GAP.



Here,  $(F/O)_{real}$  is the actual molar of fuel to oxidizer,  $(F/O)_{stoichiometric}$  is the molar of fuel to oxidizer under stoichiometric conditions

Then is the performance of the coupled mechanism on  $NO_x$  prediction is compared with the various GAP assisted  $NH_3$  combustion experimental results of Ju et al. [14] and Tang et al. [28], as shown in Fig. 4. Notably, the experimental data are all based on  $NO_x$  studies of premixed  $NH_3$ -air flames in a plasma-assisted swirl burner. For plasma-assisted ammonia/air flames, the  $NO$  peak appears around  $\phi = 0.8$  and gradually decreases as the equivalence ratio increases. Under fuel-rich conditions, the obtained  $NO$  is approximately zero. The numerical simulation results correspond well with this trend. Experimental results are well captured by the Mao-Alnasif mechanism. The deviation of the mechanism from the experiment is less than 5 % When  $\phi$  is 0.7–0.82 and 0.95–1.0.

### 3. Result and discussion

#### 3.1. Effect of GAP on density of main species

This section discusses the variation in gas density and temperature of the main components of premixed  $NH_3$ -air gas under GAP at  $E/N = 30$  Td. This  $E/N$  value is selected for analysis as it falls within the estimated range for the GAP experiments.

The transformation of gas species during the gliding arc plasma actuation can be divided into two distinct phases as shown in Fig. 5(a) and (b). The first phase involves gas ionization during the discharge phase which is up to 6.25 ms, where a high electron density facilitates collisions between high-energy electrons and gas molecules. These interactions transfer energy to the gas molecules, exciting them from their ground or low-excited states to vibrationally excited states [37]. This responds to the fact that the densities of  $NH_3$ , nitrogen ( $N_2$ ), and oxygen ( $O_2$ ) all decrease significantly during the residence time in Fig. 1. As shown in Fig. 5 (a), after plasma ionization, the final gas density of  $N_2$  and  $O_2$  decreased by 26 % and 44 % respectively. The final observed change in density is 26 % for  $N_2$  and 44 % for  $O_2$ . Furthermore, oxygen atoms present the highest percentage of H, N and O. It is presumed that this is since oxygen has a lower ionization (12.07 eV) and dissociation energy (5.12 eV) and is more easily ionized and dissociated [40]. Oxygen atoms, being chemically active, can be generated via various reaction pathways. During the discharge phase, the arc raises the gas temperature, which is further governed by the specific heat, leading to a gradual temperature increase, as shown in Fig. 5 (a). It is also observed that after the current disappears, the temperature decreases before eventually rising by approximately 100 K. Some intermediate components are generated during the plasma process as shown in Fig. 5 (b). The final gas composition of  $NH_2$  and  $OH$  has increased by 6.75 % and 4.74 %, respectively.

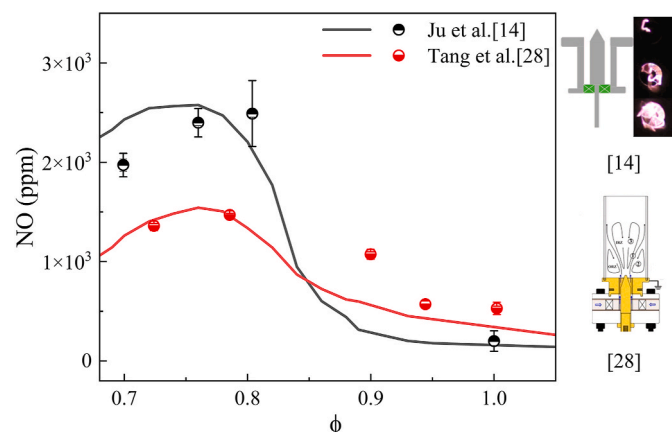


Fig. 4. Validation of  $NO$  emissions. (line: numerical, symbol: experiment).

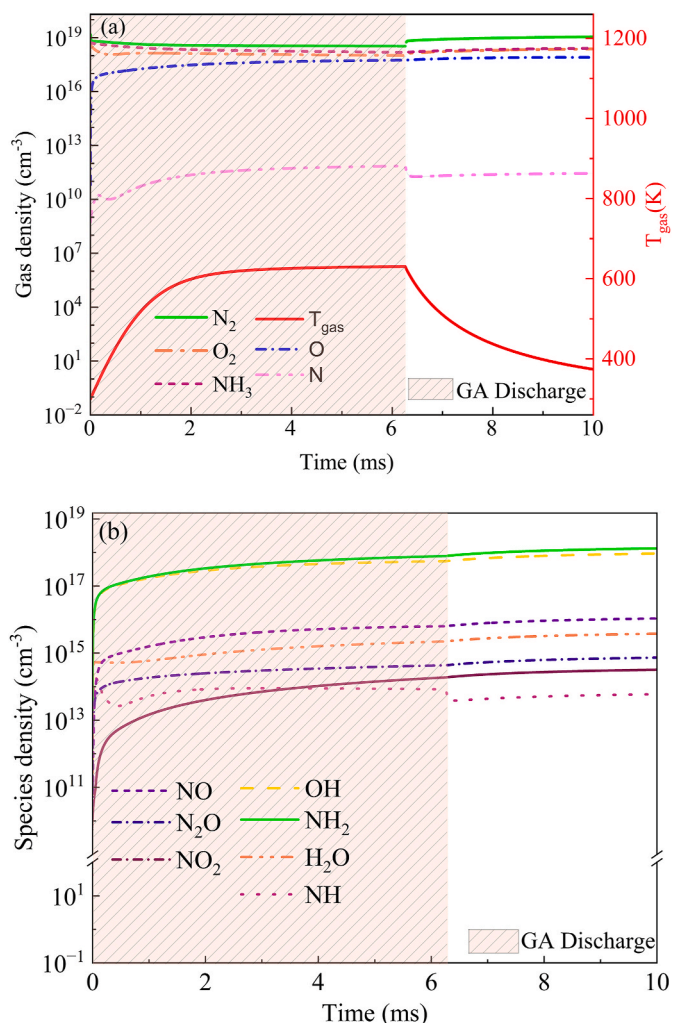


Fig. 5. Temporal evolution of species density and gas temperature for different main species. ( $\phi = 1$ ,  $T = 300$  K,  $P = 1$  atm,  $E/N = 30$  Td).

#### 3.2. Behaviour of $NH_3$ in GAP

In this section, the behaviour of  $NH_3$  ionization at different  $E/N$  is analysed and the pathways of  $NH_3$  generation and consumption with GAP is discussed.

The temporal evolution of behavioural change of  $NH_3$  during the plasma actuation are shown in Figs. 6 and 7. During the initial breakdown moment,  $NH_3$  vibrates from the ground state to different excited states. Afterwards, the different excited states of  $NH_3$  react with the initial gas components to form new  $NH_3$  molecules. It is interesting to note that the excited states generated by the main vibrations of  $NH_3$  at different energy injections (for different  $E/N$ ) are all  $NH_3(v2)$ . This is also consistent with the conclusions of Zheng et al. [37]. The rates of  $NH_3(v4)$  and  $NH_3(v13)$  production decrease slightly with increasing  $E/N$ . The generation rate is always smaller than the consumption efficiency, and the overall components show a decreasing trend. It means that in Fig. 7, the black line indicates that the reaction rate of  $NH_3$  conversion to different vibrationally excited states of  $NH_3$  is always more than the reaction rate of  $NH_3$  generation indicated by the red line.

The pathway of  $NH_3$  production and consumption is shown in Fig. 8 (a) and (b). It is observed that interconversion reactions between  $NH_3$  and different excited states of  $NH_3$  dominate the ionization phase as depicted in Fig. 8 (a). In addition to the interconversion of  $NH_3$  with different excited states, there are further modes of consumption of  $NH_3$  as shown in Fig. 8 (b). Reacting with different electronically excited

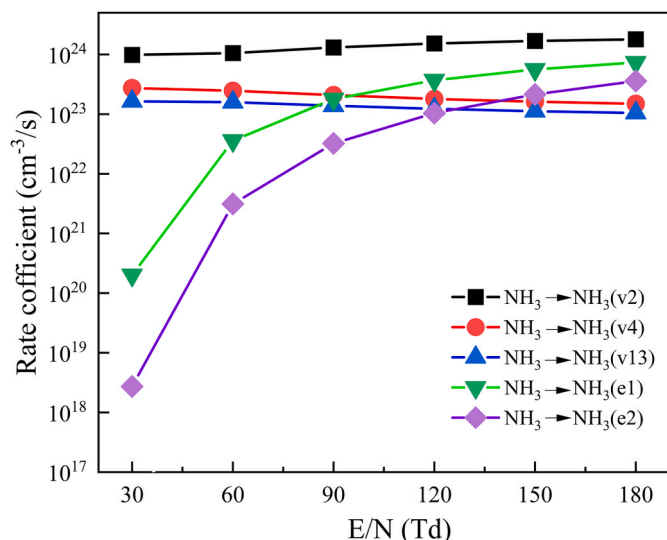


Fig. 6. Variation of electron reactions of  $\text{NH}_3$  at different  $E/N$  (30 Td-180 Td).

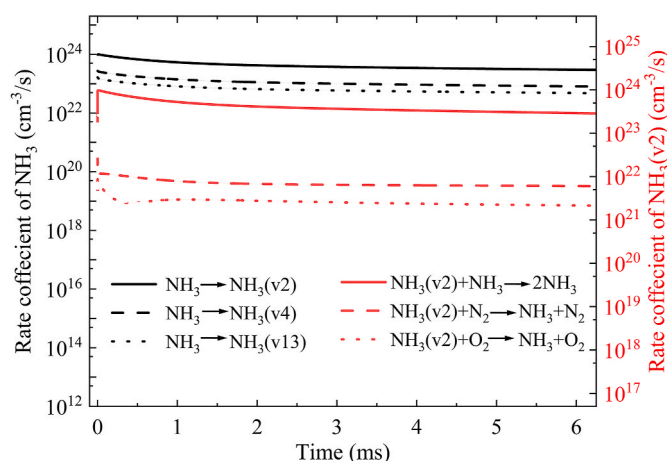


Fig. 7. Variation of rate coefficients of  $\text{NH}_3$  and vibrationally excited state  $\text{NH}_3$  during the GA discharge time at 30 Td.

states of  $\text{N}_2$ , nitrogen and oxygen atoms, dehydrogenate to form  $\text{NH}_2$ . This is one of the reasons for the higher production of  $\text{NH}_2$  mentioned in 3.1. In parallel, the rate of reaction to produce is more significant in the discharge phase than in the no-discharge phase.

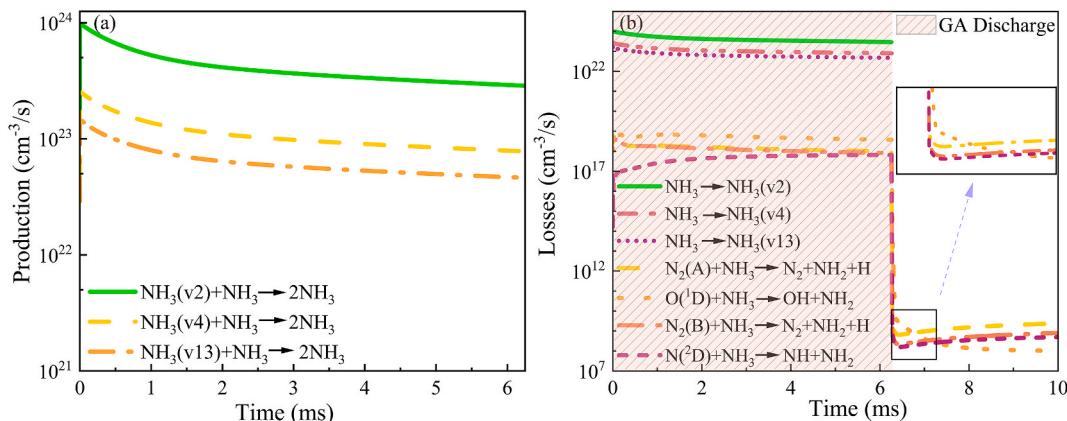


Fig. 8. (a) Production and (b) losses of  $\text{NH}_3$  under GAP.

### 3.3. Generation of main groups affecting NO production

In this section, major radicals such as OH, NH, and  $\text{NH}_2$  for NO generation and consumption with different  $E/N$  are discussed. This was taken as the reason for analysing the reduction in NO emissions when GAP promotes  $\text{NH}_3$ -air combustion.

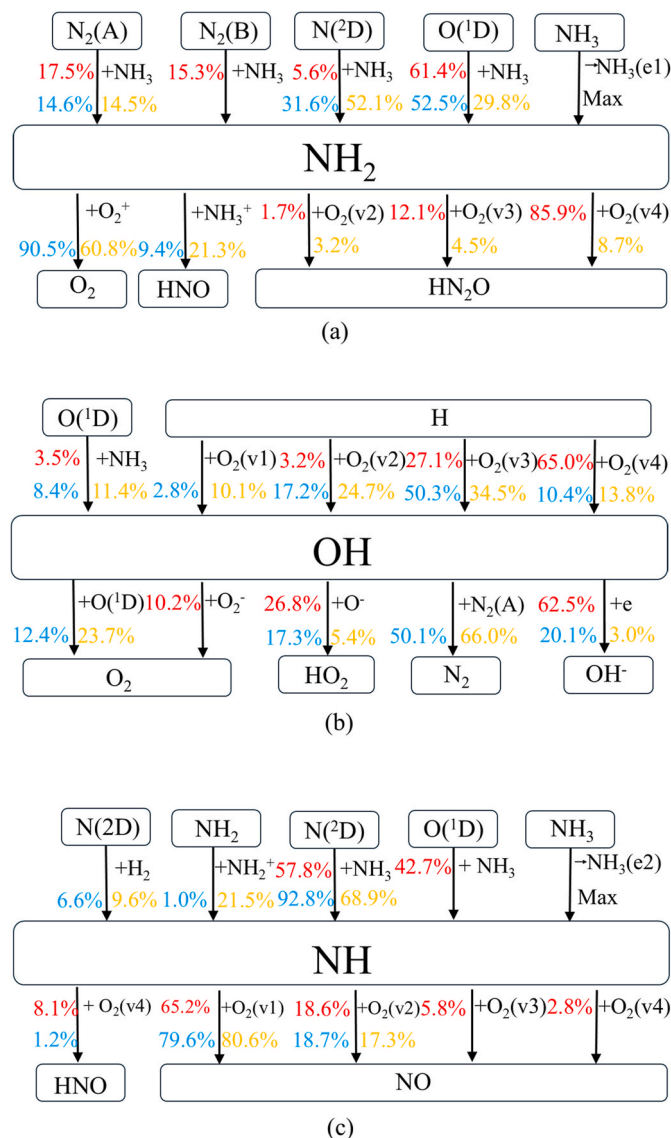
The sensitivity analyses of the groups (OH, NH,  $\text{NH}_2$ ) that play a primary role in NO production/consumption with plasma are shown in Fig. 9. According to Fig. 9 (a) and (c),  $\text{NH}_2$  and NH, as the main pathways for NO consumption, show the strongest sensitivities to the reactions from  $\text{NH}_3$  to  $\text{NH}_3(\text{e}1)$  and  $\text{NH}_3(\text{e}2)$ , respectively. The electron collision reactions of  $\text{NH}_3$  as affected by the strength of the electric field showed that the rate of the reaction to produce  $\text{NH}_3$  in the different excited states increased rapidly with an increased  $E/N$  as illustrated in Fig. 6. This indicates that high field strength helps to promote the consumption path of NO. For the  $\text{NH}_2$  generation reaction, the  $\text{O}(^1\text{D}) + \text{NH}_3 \rightarrow \text{OH} + \text{NH}_2$  and  $\text{N}_2(\text{A}) + \text{NH}_3 \rightarrow \text{NH}_2 + \text{N}_2 + \text{H}$  reaction dominates (30 Td). As  $E/N$  increases,  $\text{N}(^2\text{D}) + \text{NH}_3 \rightarrow \text{NH}_2 + \text{H} + \text{N}_2$  gradually takes the lead (52.1 % in 90 Td). Under low-temperature conditions, the thermal motion of molecules is reduced, and chemical reactions primarily rely on non-thermal processes (such as electron impact or the involvement of excited species).  $\text{N}(^2\text{D})$  and  $\text{O}(^1\text{D})$  loses energy through collisions with surrounding molecules or energy transfer, leading to the generation of intermediate radicals (e.g., OH and  $\text{NH}_2$ ) [23]. Nevertheless, the increase of OH is often accompanied by the generation of NO, through HNO reactions. In Fig. 9 (b), the main pathway of OH formation is the reaction between H atoms and oxygen in different vibrational excited states.

### 3.4. Effect of GAP on combustion characteristics

In this section, sensitivity analyses and reaction pathways of NO in  $\text{NH}_3$ -air combustion under GAP were investigated. Previous experiments have shown that the maximum  $\phi$  of NO change with plasma is between 0.8 and 0.9 [14,32], so this  $\phi$  was selected for the present analysis.

The sensitivity analysis under plasma-assisted combustion versus pure combustion with path flux of NO is shown in Figs. 10 and 11. The sensitivity of plasma assisted combustion at different  $\phi$  is approximately the same for the different reactions, the maximum sensitivity coefficients all occur in the reaction of HNO with H as shown in Fig. 10. The two reactions that consume NO show a significant magnitude of rate due to the generation of  $\text{NH}_2$  and NH. The reaction  $\text{N} + \text{NO} = \text{N}_2 + \text{O}$  at  $\phi = 0.8$  and 0.9 with sensitivity coefficients of 0.91 and 0.98. The rate increases due to the increase in N atoms produced by ionization, which contributes more to the consumption of NO.

Diversification of NO consumption paths at different  $\phi$  (reactions  $\text{NH} + \text{H} = \text{N} + \text{H}_2$ ,  $\text{HNO} + \text{OH} = \text{NO} + \text{H}_2\text{O}$ ) attributed to plasma-generated intermediate groups. Similarly, in Fig. 11, combustion with or without



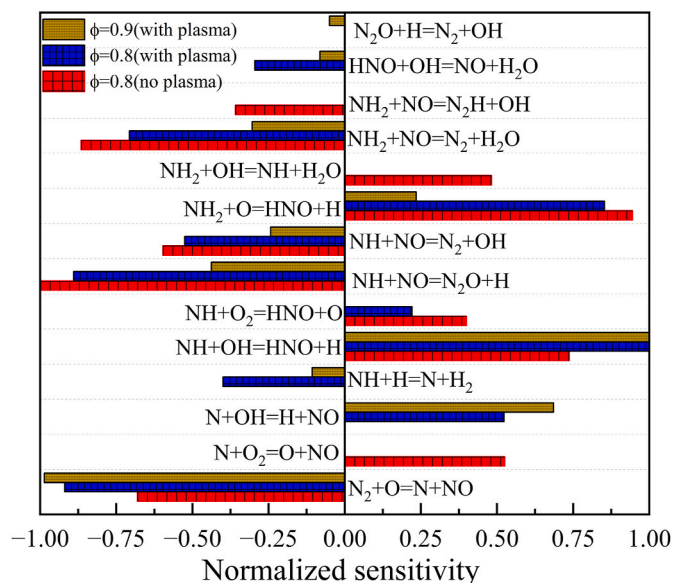
**Fig. 9.** Sensitivity analysis of (a) NH<sub>2</sub> (b) OH and (c) NH on the NO production at 30(red), 60(blue), 90(orange)Td in plasma. (Numbers indicate the total reaction percentage). (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

plasma, HNO is the main pathway for NO production, the same as that of literature [16,41]. Almost 50 % of NO is produced through the pathway of HNO with and without plasma. The percentage rate of production of NO consumed by NH<sub>2</sub> in GAP (12.9 %) is about twice as high as without GAP (5.9 %). Meanwhile, OH and N atoms are produced during the ionization phase, leading to the reaction OH + N = H + NO exacerbated by NO production with GAP (14.4 %, compared with 8.7 % without GAP).

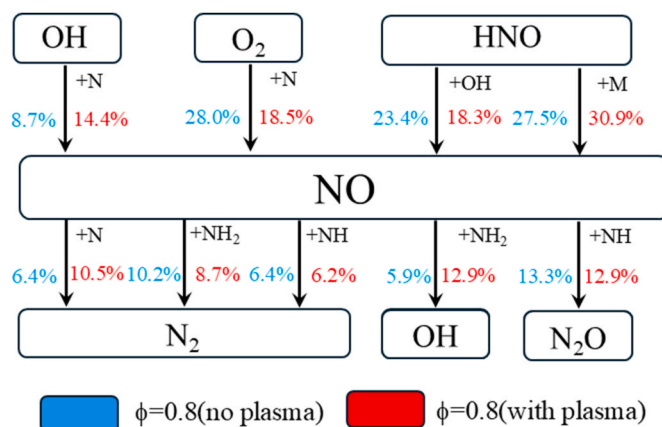
#### 4. Conclusion

This study presents a numerical model for predicting NO<sub>x</sub> emissions during gliding arc plasma (GAP)-assisted combustion of an NH<sub>3</sub>-air mixture. The NO production and consumption mechanisms under GAP actuation in NH<sub>3</sub>-air mixtures are also investigated in detail. The main conclusions are summarized below:

- (1) Three plasma reaction mechanisms for NH<sub>3</sub>-air combustion were compared with the present GAP experiment. The mechanism of



**Fig. 10.** Sensitivity analysis of NO production and consumption at  $\phi = 0.8$  and 0.9.



**Fig. 11.** Path flux of NO emissions at  $\phi = 0.8$  (with plasma and no plasma).

Mao et al. [23] was found to be optimal and was subsequently coupled with the Alnasif et al. [38] optimized combustion mechanism to develop a plasma-assisted combustion model.

- (2) The results revealed that NO production primarily occurs via the HNO pathway, regardless of GAP actuation. The GAP Plasma reduces NO primarily by breaking down NH<sub>3</sub> into NH<sub>2</sub> (6.75 % in 30 Td), which enhances NO consumption, mainly through N<sub>2</sub>(A) + NH<sub>3</sub> → NH<sub>2</sub> + N<sub>2</sub> + H and O(<sup>1</sup>D) + NH<sub>3</sub> → OH + NH<sub>2</sub>.
- (3) It is observed that higher plasma power further facilitates NO consumption. Strong electric fields promote the generation of excited ammonia states, which exhibit a higher tendency to form NH<sub>2</sub> and NH, enhancing NO reduction. NH<sub>2</sub> showed high sensitivity (52.1 %) to the reaction N(<sup>2</sup>D) + NH<sub>3</sub> → NH<sub>2</sub> + H + N<sub>2</sub>, N<sub>2</sub>(A) + NH<sub>3</sub> → NH<sub>2</sub> + N<sub>2</sub> + H. NH showed high sensitivity (68.9 %) to the reaction N(<sup>2</sup>D) + NH<sub>3</sub> → NH<sub>2</sub> + NH (90 Td).

Future studies should take into account the influence of the swirling flame structure, the propagation of the arc within the GAP particularly the impact of arc rotation on spatial variations as well as other factors that may affect flame behaviour.



## CRediT authorship contribution statement

**Ziyu Wang:** Writing – original draft, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **B. Aravind:** Writing – review & editing, Supervision, Methodology, Investigation, Conceptualization. **Syed Mashruk:** Writing – review & editing, Supervision. **Agustin Valera-Medina:** Writing – review & editing, Supervision, Funding acquisition.

## 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 data to this article can be found online at <https://doi.org/10.1016/j.joei.2025.102314>.

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