

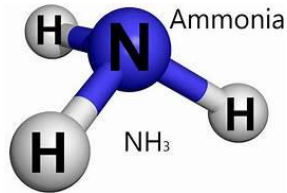


UNIVERSITÀ  
DEL SALENTO



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***Title: Ammonia and ammonia/hydrogen mixtures  
combustion associated with plasma***



**Winter Hydrogen School  
8-12<sup>th</sup> January**

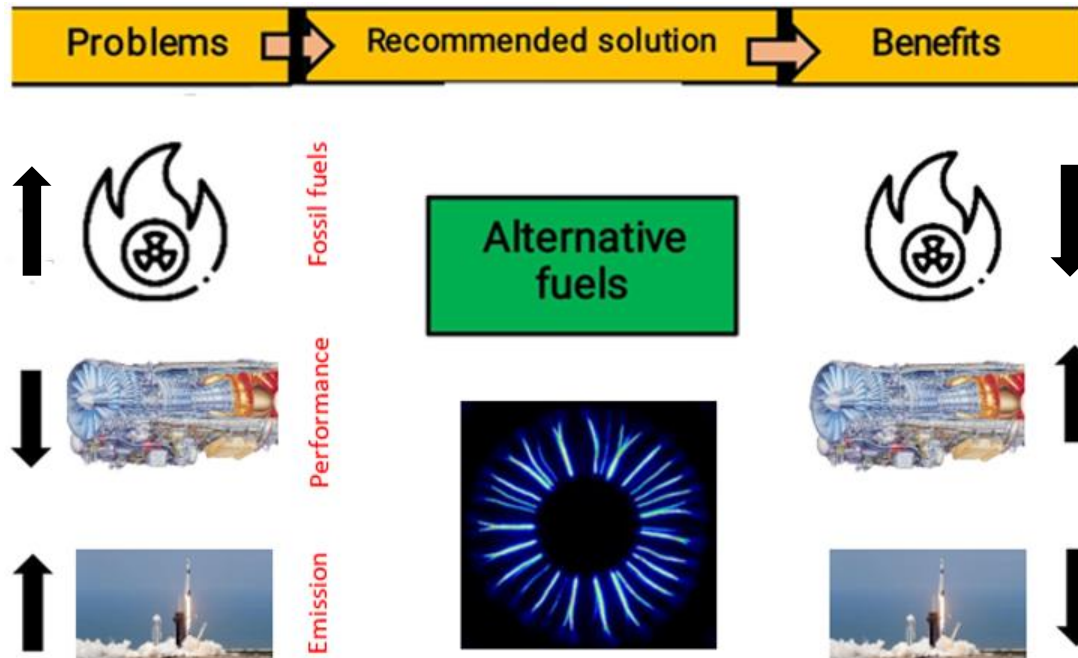
**Presented By: Zubair Ali Shah**

**Department of Engineering for Innovation,  
University of Salento, Italy**



# Motivation and background

- **Combustion** is the principal energy conversion method for electricity generation and transportation since the industrial revolution. To this day, these sectors significantly rely on **fossil fuels**.



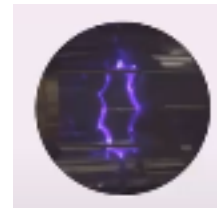
# Motivation and background

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- Plasma Associated Combustion (PAC) is the prominent and active control technology to **boost combustion** and **minimize pollutant emissions** by controlling **combustion instability**.
- Enhancement of the combustion of **Hydrocarbons**



Ignition in IC engine,  
Scramjet...



Burning velocity  
of laminar and  
turbulent flames...

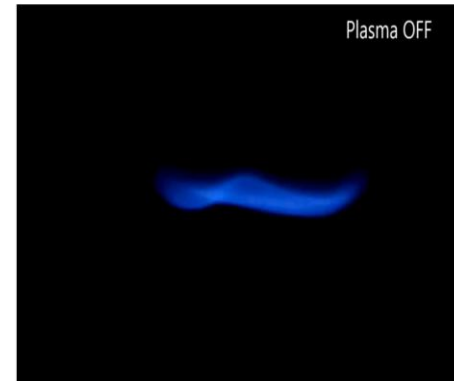
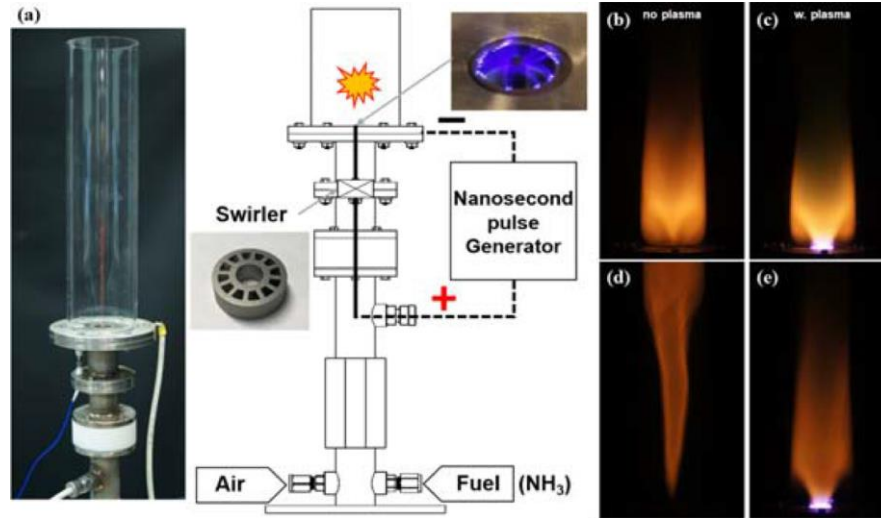


Lean blow-off and  
stability limits



Control of  
thermoacoustic  
instabilities

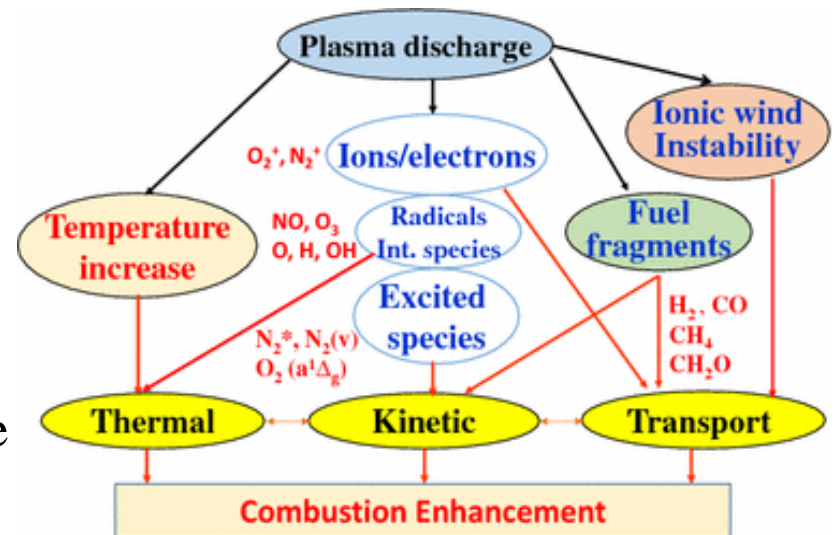
# Motivation and background



# Motivation and background

❖ Plasma assisted combustion technology has the potential to enhance combustion by:

- **Thermal effect** via temperature rise
- **Kinetic effect** via plasma generated **electronically** and vibrationally excited molecules and active radicals
- **diffusion transport enhancement effect** via fuel decomposition and low temperature oxidation



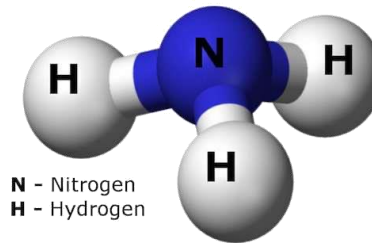
Plasma-generated **ionic wind**, and **flow motion**, via the Coulomb and Lorentz forces, which **increase turbulization, mixing** and alters local flow velocity.

# Challenges with ammonia combustion

## ❖ Ammonia combustion Merits & Drawbacks

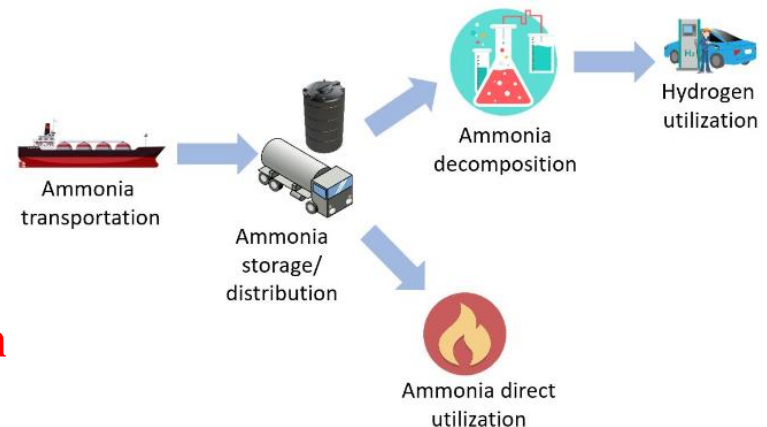
### ➤ Merits

- High hydrogen density
- Carbon free nature
- Good infrastructure



### ➤ Drawbacks

- Poor ignition timings
- Lower burning velocity
- Shorter flammability limits and
- High  $\text{NO}_x$  emissions

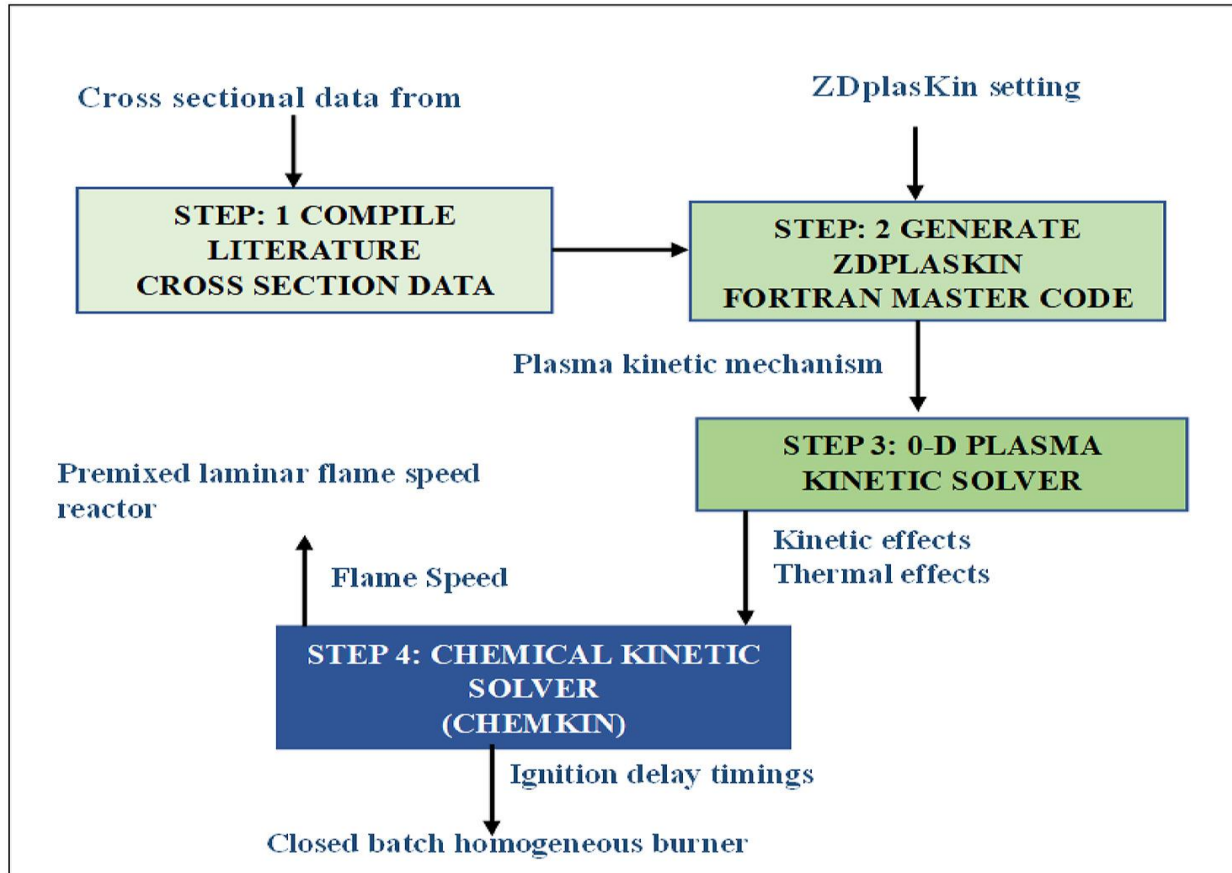


# Aims and objectives

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- To develop detailed and comparative numerical **combustion and plasma chemical kinetic mechanisms** to analyze the combustion of alternative fuels (Ammonia, Hydrogen, etc.).
  - Experimental **Validation of newly developed mechanisms.**
  - Parametric study of different parameters to obtain the optimum conditions for **flame speed, ignition delay time, flame stability** and **pollutant emission.**
  - Perform the experiments with and without **plasma** to investigate the **effect** of key parameters (Temperature, pressure, reduced electric field, equivalence ratio, etc.) on ammonia and hydrogen fuels combustion.
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# Plasma Assisted Combustion– Methodology



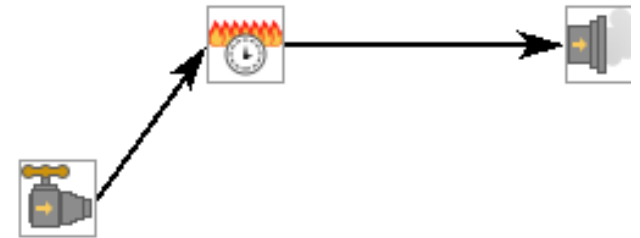
A detailed sketch of the numerical coupling of ZDPlasKin and CHEMKIN.



# Plasma and Combustion Kinetic mechanism Details

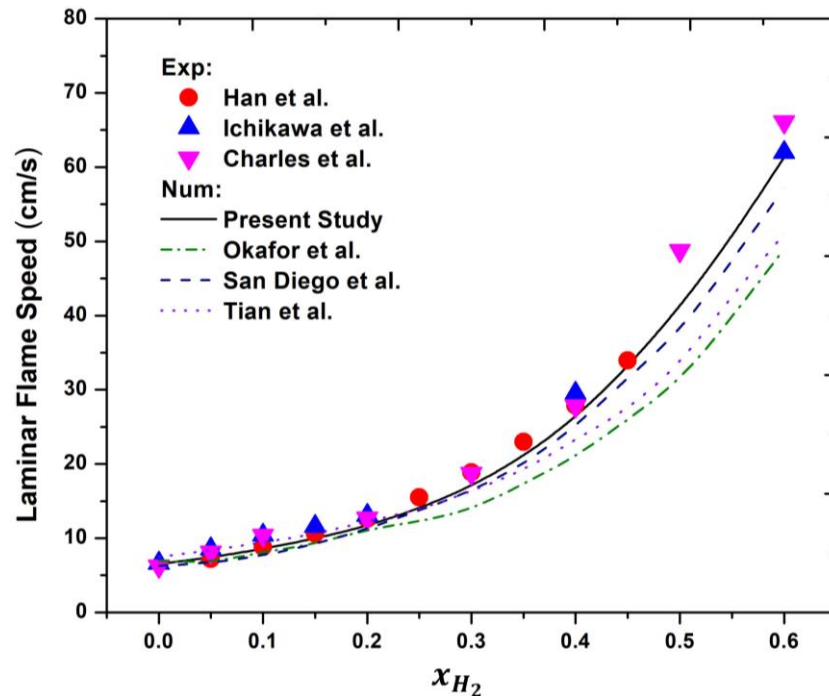
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- The new kinetic reaction mechanism used for the combustion simulation in CHEMKIN is developed.
- For the modeling of laminar flame speed (LFS) and ignition delay time (IDT), premixed laminar flame speed reactor (PLFSR) and 0D Close Homogeneous Batch Reactor (CHBR), respectively were used.

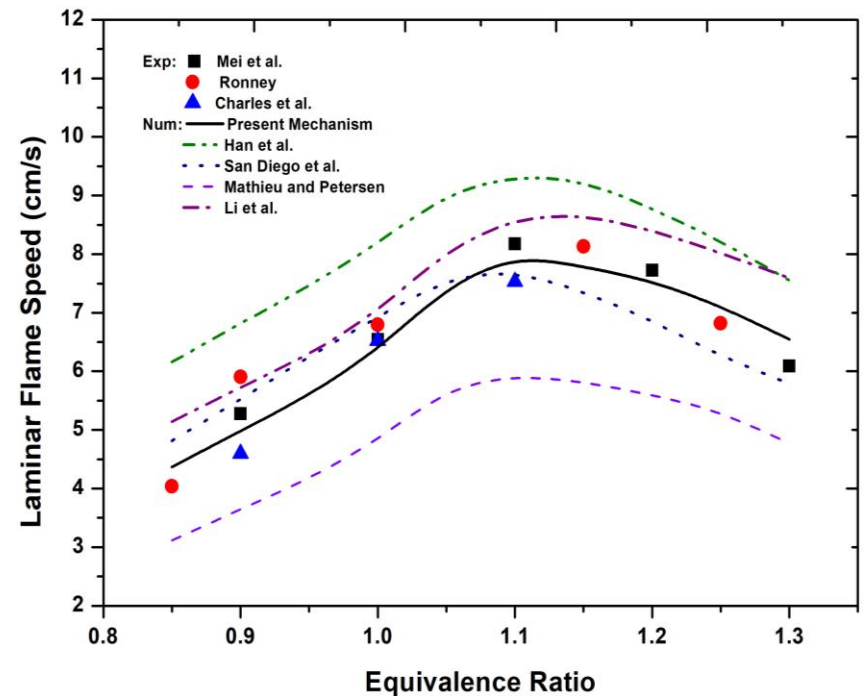


# Combustion Kinetic mechanism Validation

## ❖ Kinetic Mechanism Validation

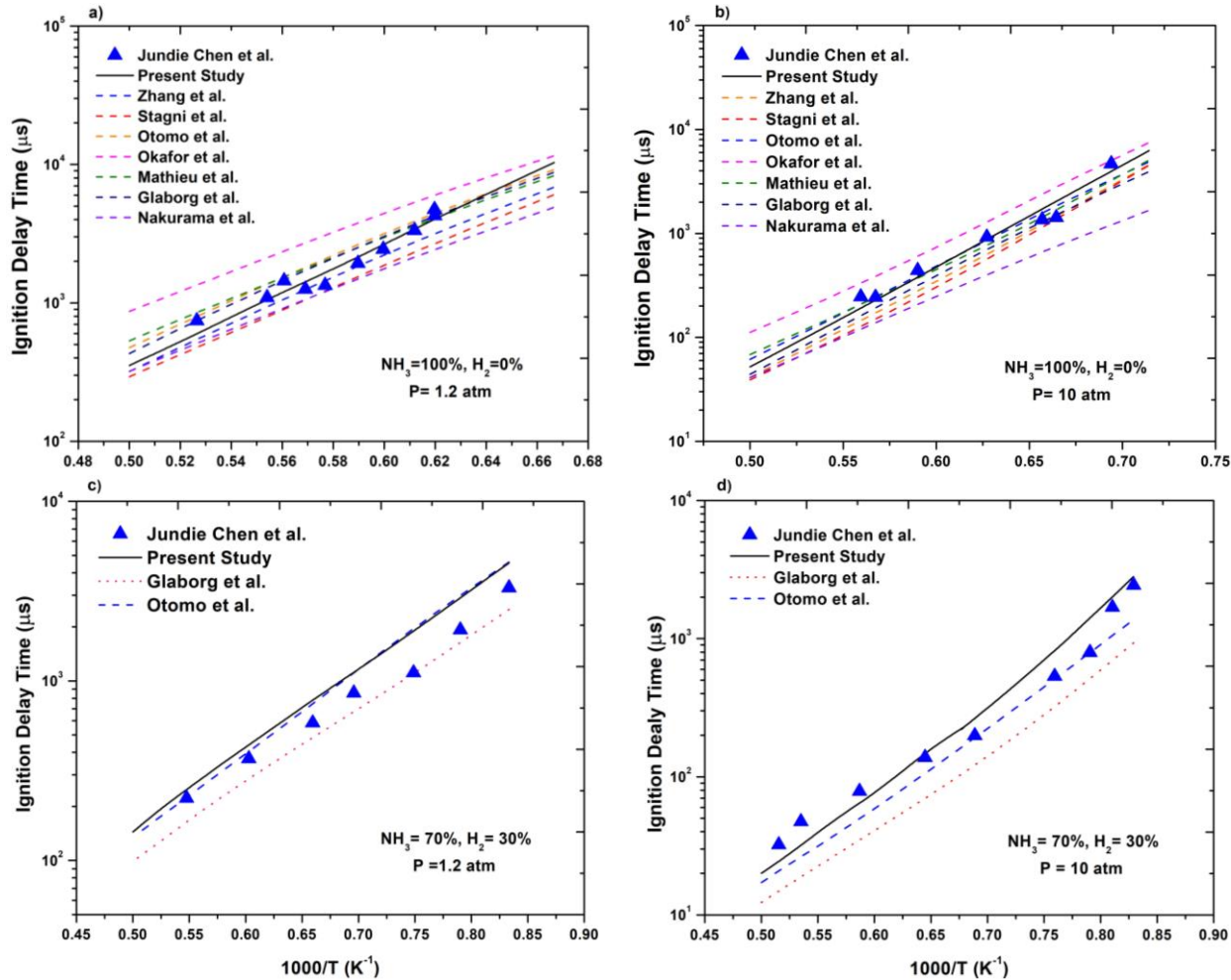


LFS of stoichiometric  $\text{NH}_3/\text{H}_2/\text{air}$  mixtures, as a function of  $x_{H_2}$ . Symbols signify the experiment data, whereas lines show the simulated findings of the current model and prior models at  $P=1\text{atm}$  and  $T=298\text{K}$ .



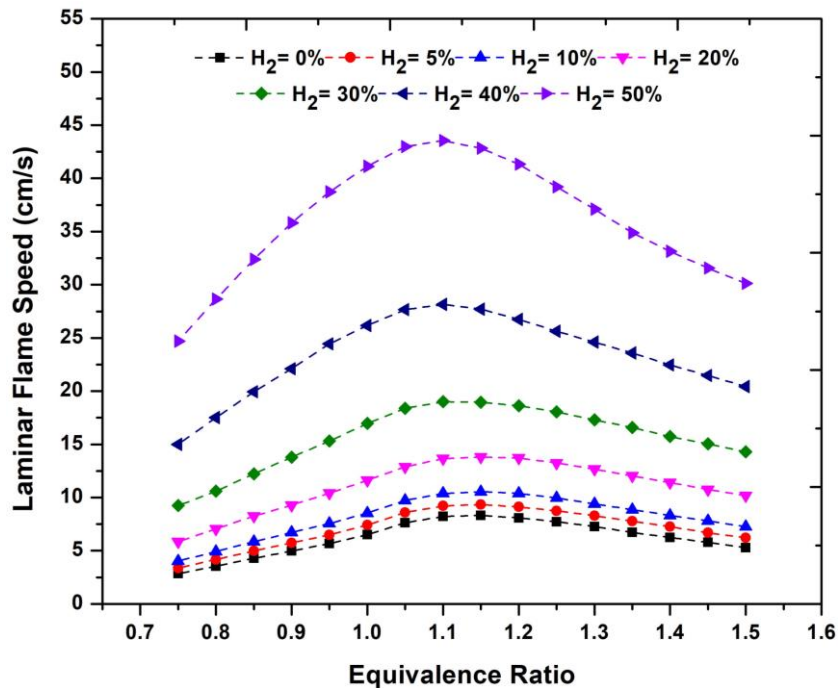
LFS of  $\text{NH}_3/\text{air}$  flame at standard conditions. Symbols signify the experiment data and lines show the simulated findings of the current model and prior models.

# Combustion Kinetic mechanism Validation

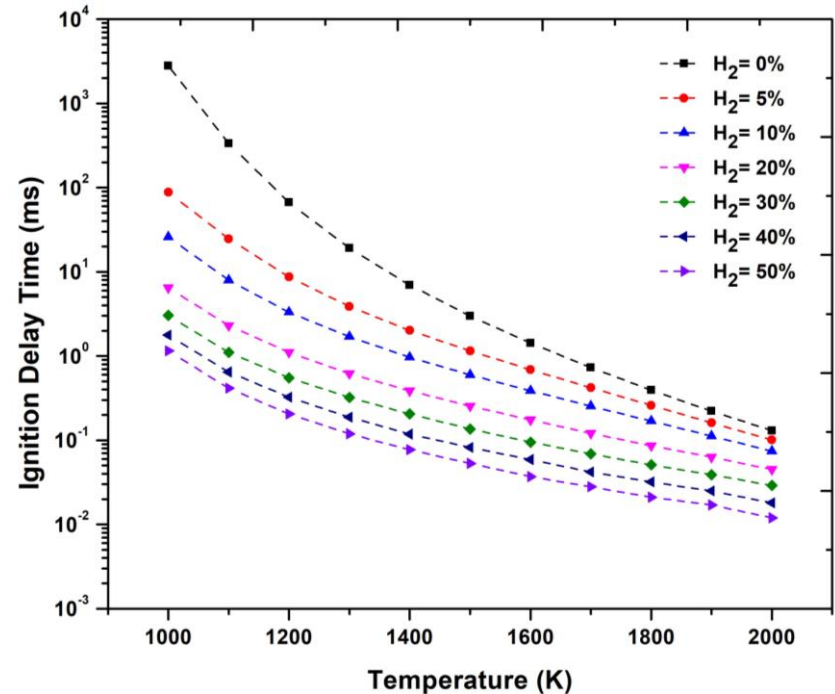


# Results and Discussion

## ❖ Effect of Hydrogen Enrichment in the $\text{NH}_3/\text{Air}$ Mixture on LFS & IDT



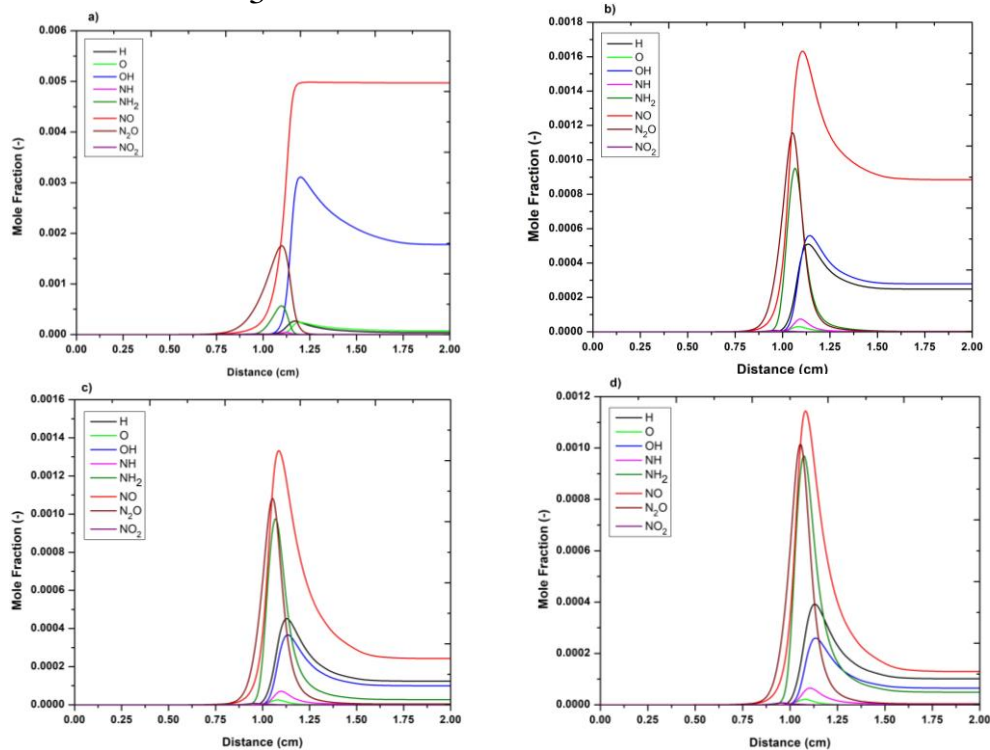
Effect of hydrogen enrichment and equivalence ratio of  $\text{NH}_3/\text{air}$  mixtures on the LFS at  $P = 1$  atm and  $T = 298\text{K}$



Effect of Hydrogen enrichment of  $\text{NH}_3/\text{air}$  mixtures on IDT at  $\Phi = 1$ ,  $P = 1$  atm.

# Results and Discussion

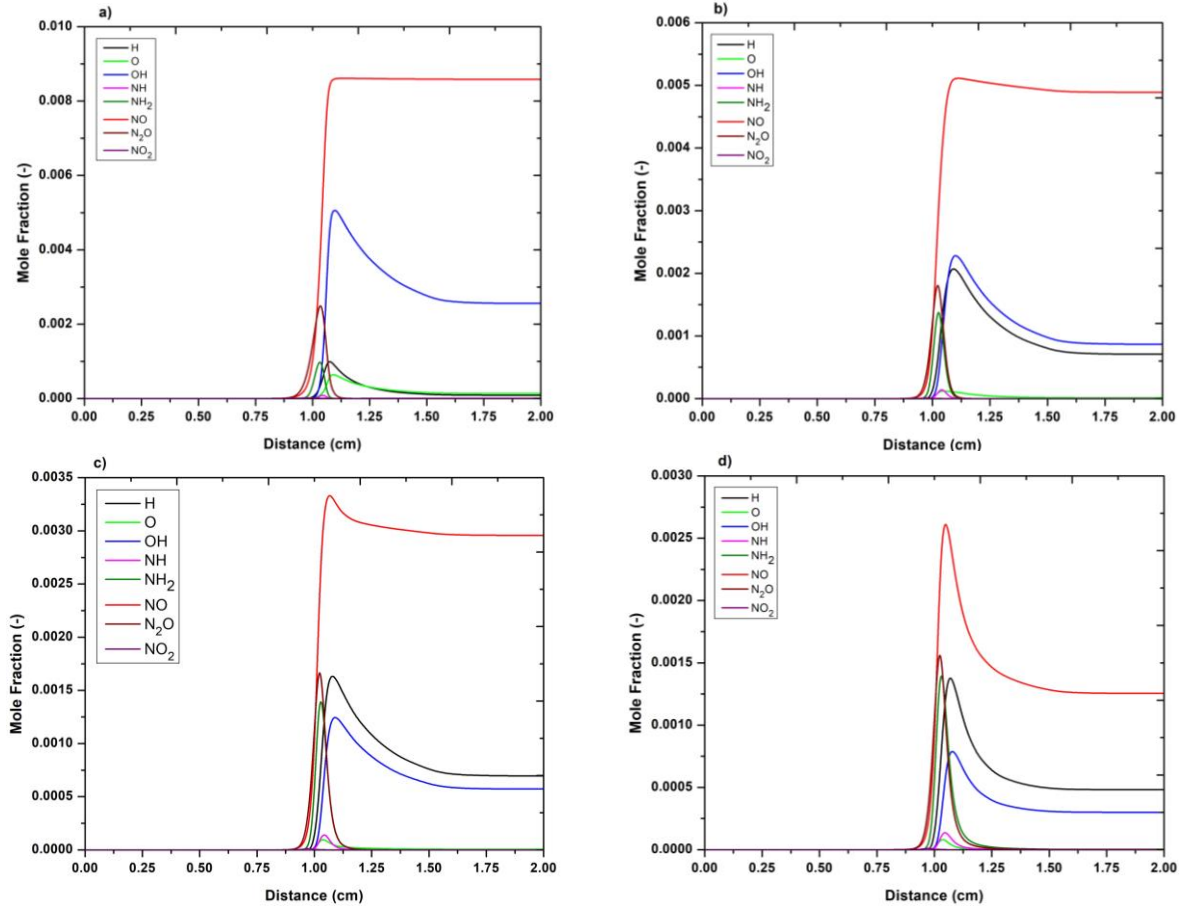
- ❖ The effect of **blending hydrogen** and **equivalence ratio** on the **mole fraction profiles species** of  $\text{NH}_3$  /air mixture



Mole fraction profiles of H, O, OH, NH<sub>2</sub>, NH, NO, N<sub>2</sub>O & NO<sub>2</sub> of  $\text{NH}_3$ /air mixtures at different equivalence ratios a)

$\Phi = 0.9$  b)  $\Phi = 1.1$  c)  $\Phi = 1.15$  d)  $\Phi = 1.2$ , and  $P = 1$  atm and  $T = 298\text{K}$

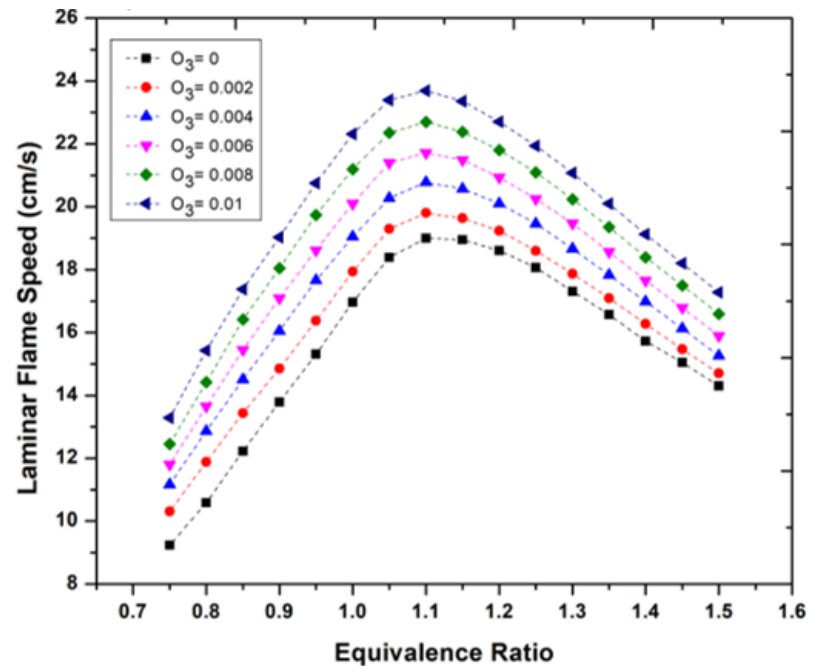
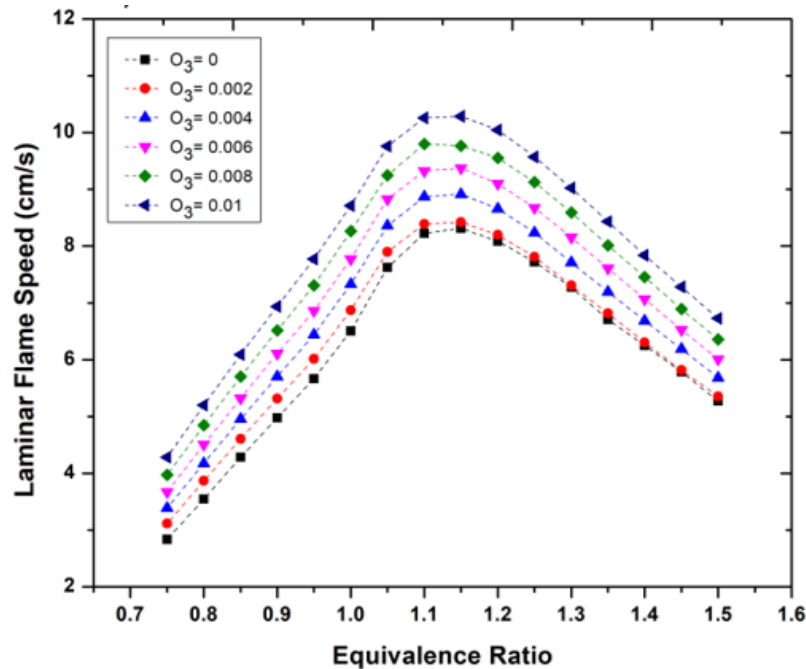
# Results and Discussion



Mole fraction profiles of H, O, OH, NH<sub>2</sub>, NH, NO, N<sub>2</sub>O & NO<sub>2</sub>, H<sub>2</sub> added 30% NH<sub>3</sub>/air mixtures at different equivalence ratios a)  $\Phi = 0.9$  b)  $\Phi = 1.1$  c)  $\Phi = 1.15$  d)  $\Phi = 1.2$  and P=1 atm T=298K

# Results and Discussion

## ❖ Effect of Ozone Enrichment in the NH<sub>3</sub>/H<sub>2</sub>/Air Mixtures on LFS

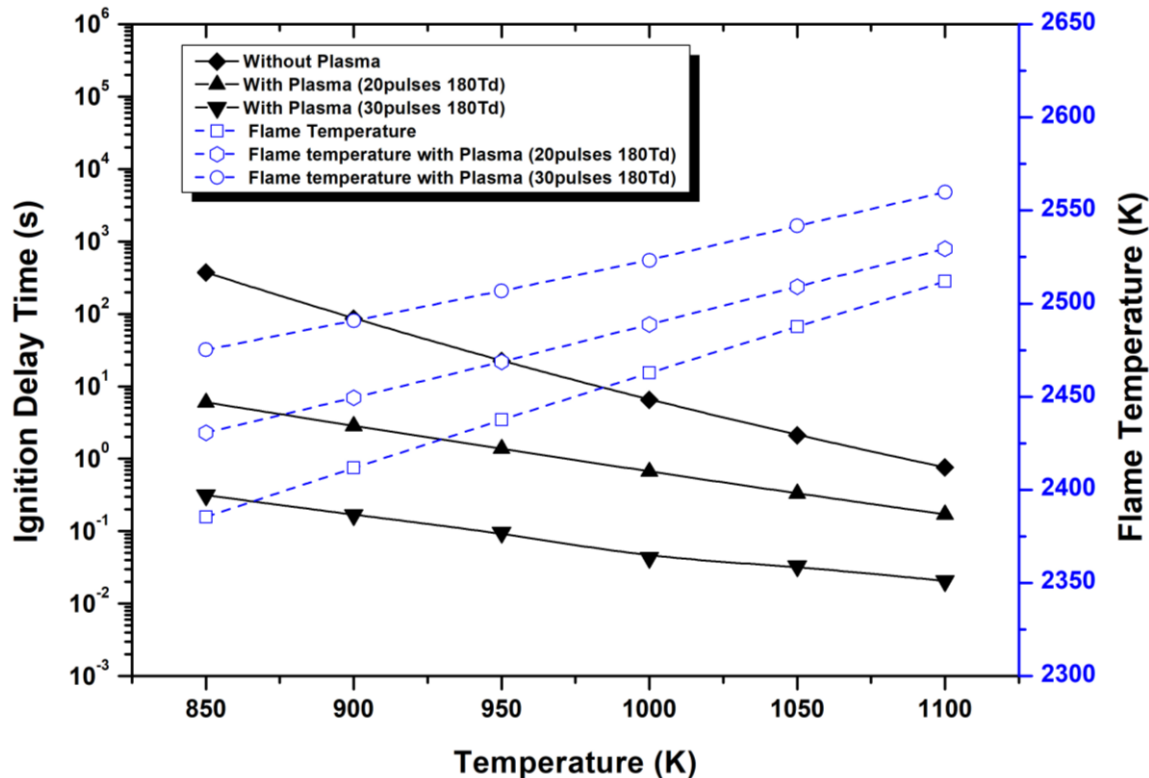


The effect of O<sub>3</sub> on LFS of NH<sub>3</sub>/H<sub>2</sub>/air mixtures under the normal condition at

H<sub>2</sub> = 0% and H<sub>2</sub> = 30%

# Results and Discussion

- ❖ Effect of **temperature** and **plasma** on IDT and flame temperature



IDT and flame temperature without and with 20 and 30 sequential pulses of plasma discharge in  $\text{NH}_3/\text{air}$  mixture at  $\phi = 1.0$  with PRF = 50 kHz.



# Conclusion

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- Laminar Flame speed increased as **H<sub>2</sub> concentration** increased, and IDT is reduced with an increased concentration of H<sub>2</sub>, and initial temperature.
  - The **optimized equivalence ratio** exists in the range of **1.10–1.15** to achieve steady and **efficient combustion** as well as **reduced NOx emissions**.
  - **The ignition delay** time of the combustion under the **plasma case** is significantly shorter and the flame temperature higher than that of the **without plasma case**. The findings suggest that plasma excitation accelerate reactions and introduces new pathways, which improves low-temperature NH<sub>3</sub> ignition.
  - Adding **ozone** in the oxidizer also can improve the LFS of the NH<sub>3</sub>/H<sub>2</sub>/air mixture at normal conditions.
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# Publications

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1. **Zubair Ali Shah**, G. Mehdi, P.M. Congedo, D. Mazzeo, M.G. De Giorgi. A review of recent studies and emerging trends in plasma-assisted combustion of ammonia as an effective hydrogen carrier. **International Journal of Hydrogen Energy** (2023) <https://doi.org/10.1016/j.ijhydene.2023.05.222>
2. **Zubair Ali Shah**, G. Marseglia, Maria Grazia De Giorgi. Predictive Models of Laminar Flame Speed in  $\text{NH}_3/\text{H}_2/\text{O}_3/\text{Air}$  Mixtures Using Multi-Gene Genetic Programming Under Varied Fuelling Conditions. **Fuel** (2023) (Under review).
3. **Zubair Ali Shah**, Mingming Zhu, Ghazanfar Mehdi, Maria Grazia De Giorgi. Refined Kinetic Mechanism for Modeling Improved Ignition Delay Time in Ammonia/Air Mixture through Nanosecond Plasma Discharge. The Combustion Institute's **40th International Symposium** - Emphasizing Energy Transition (Under review).
4. Ghazanfar Mehdi, Maria Grazia De Giorgi, Sara Bonuso, **Zubair Ali Shah**, Giacomo Cinieri and Antonio Ficarella. Comparative Analysis of Flame Propagation and Flammability Limits of  $\text{CH}_4/\text{H}_2/\text{Air}$  Mixture with or without Nanosecond Plasma Discharges. **Aerospace** 2023, 10(3), 224. <https://doi.org/10.3390/aerospace10030224>

# Publications

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5. Giacomo Cinieri, **Zubair Ali Shah**, Guido Marseglia, Maria Grazia De Giorgi. Towards Zero Carbon Emissions: Investigating the Combustion Performance of Shaped Micro-Combustors using H<sub>2</sub>/Air and NH<sub>3</sub>/Air Mixtures. Aerospace 2024, 11(1), 12; <https://doi.org/10.3390/aerospace11010012>
6. Sara Bonuso, Pasquale Di gloria, Guido Marseglia, Ramón A. Otón-Martínez, Ghazanfar Mehdi, **Zubair Ali Shah**, Antonio Ficarella, Maria Grazia De Giorgi. Investigation into the effect of Hydrogen-Enriched Conditions on Methane Flame Structure and Stability. Aerospace 2024, 11(1), 43; <https://doi.org/10.3390/aerospace11010043>
7. Sara Bonuso, Ghazanfar Mehdi, **Zubair Ali Shah**, Maria Grazia De Giorgi. Experimental Investigation of the Effect of Hydrogen Enrichment on Flame Structures: Insights into Flame Characteristics and Stability. 13th EASN International Conference Proceedings Issue of Journal of Physics (2023) (**Accepted**).
8. G. Cinieri, G. Marseglia, **Zubair Ali Shah**, Ghazanfar Mehdi, M.G. De Giorgi. Combustion Performance of Zero-carbon Fuels in a Shaped Micro-Combustor for Aerospace Propulsion Applications. 13th EASN International Conference Proceedings Issue of Journal of Physics (2023) (**Accepted**).

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**Thank you**  
**For your Attention**

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