수소 혼합에 따른 암모니아 확산 화염의 구조 및 NO_X 배출 특성 분석

Effect of Hydrogen Addition on Flame Structure and NOX Emission Characteristics in Laminar Ammonia Diffusion Flames

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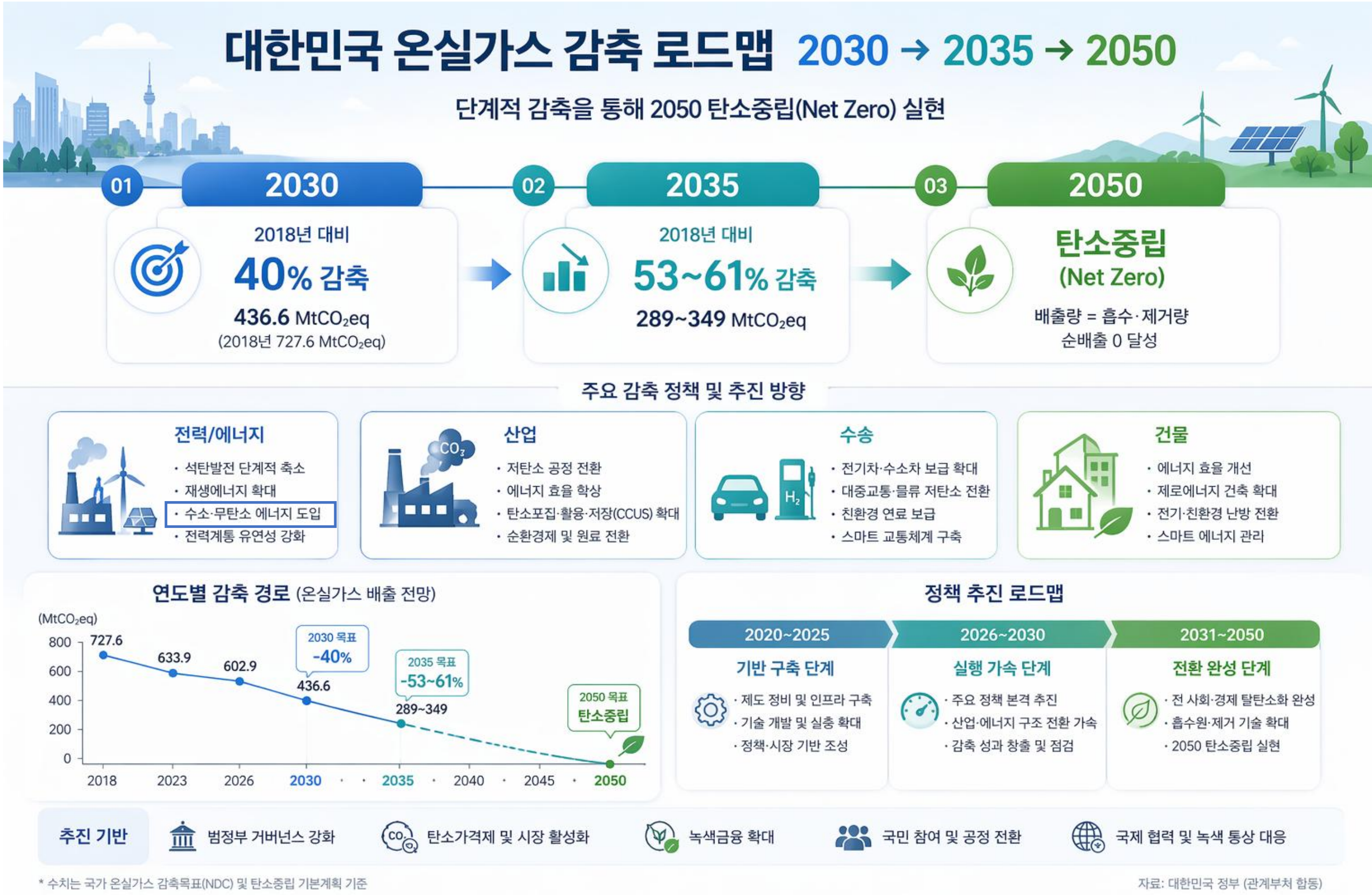
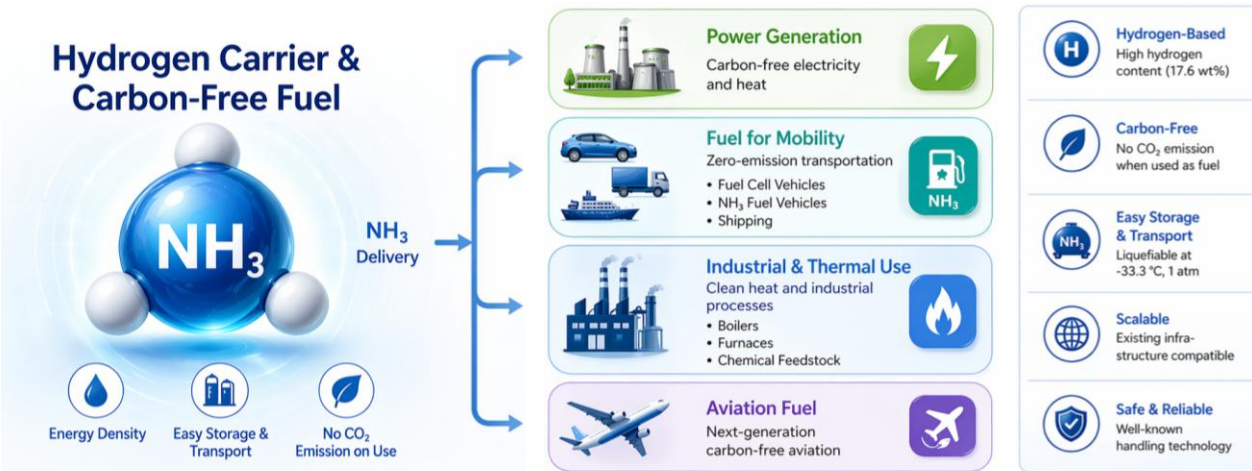
Korea's Carbon Neutrality Roadmap (2030 – 2050)



Clean Energy Applications of Ammonia(NH_3)



KEY CHALLENGES

Difficulty in Ignition

- Low reactivity
- High ignition energy

Flame Instability

- Low flame speed
- Susceptible to blowoff

Combustion Characteristics of NH_3

Ammonia combustion and emssions in practical applications.., Mohammad Alnajideen et al, *Carbon Neutrality*, 2024

- Low chemical reactivity
  → Slow reaction kinetics and low LBV
- Low flame temperature (compared to H_2 or C_mH_n)
- Narrow flammability range
  → Difficult to sustain stable combustion
- High ignition energy
  → Requires strong ignition source

▪ Table 1 Properties of NH_3 and common fuels

	NH_3	H_2	CH_4	C_3H_8
LHV(MJ/kg)	18.6	120.0	50.0	46.4
Flammability limit (φ)	0.63 – 1.4	0.10 – 7.1	0.50 – 1.7	0.51 – 2.5
Adiabatic flame temp.(^oC)	1800	2110	1950	2000
Auto-ignition temp. (^oC)	650	520	630	450
Max. LBV(m/s)	0.07	2.91	0.38	0.43
Min. ignition energy (MJ)	8.00	0.02	0.28	0.25

NO_X Formation Pathways

NO_X Emission and Control in Ammonia Combustion : State-of.., Xuren Zhu et al, *Energy & Fuels*, 2024

- NH_3 decomposition

  $NH_3 + H \rightarrow NH_2 + H_2$

  $NH_3 + OH \rightarrow NH_2 + H_2O$

- Fuel NO pathway

  $NH_2 + O \rightarrow NH + OH$

  $NH + O \rightarrow NO + H$

  $NH + OH \rightarrow HNO + H$

- Thermal NO pathway

  $N_2 + O \rightarrow NO + N$

  $N + O_2 \rightarrow NO + O$

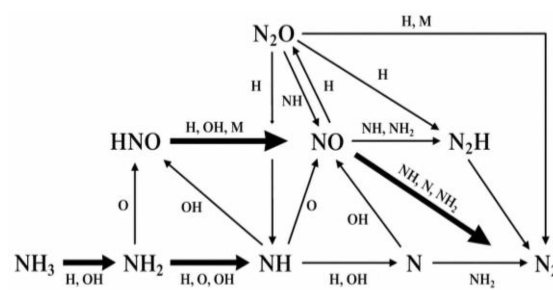
  $N + OH \rightarrow NO + H$

- N_2O to NO or N_2 pathway

  $N_2O + O \rightarrow 2NO$

  $N_2O + H \rightarrow N_2 + OH$

  $N_2O + OH \rightarrow N_2 + HO_2$



Enhancement of NH_3 Combustibility

Through fuel preheating

Effect and mechanism of combustion enhancement and emission reduction.., Yifeng Chen et al, *Fuel*, 2022

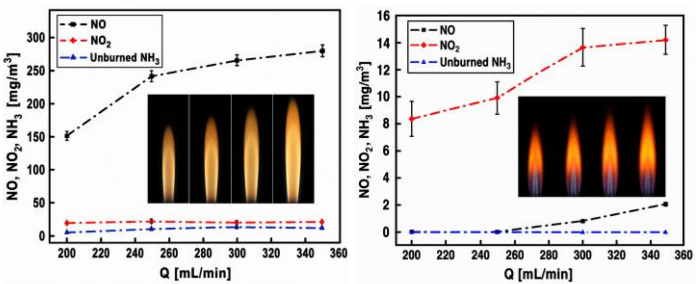


Fig.1 variation in emissions(NO, NO_2, unburned NH_3) with different NH_3 flow rates (left : 593 K right : 773 K)

- Increasing preheating temperature,
  - Enhances NH_3 reactivity.
  - Flame stability improves.
  - Unburned NH_3 significantly decreases.
- At high preheating temperature,
  - NO emission decreases.
  - NO_2 becomes the dominant NO_X.

In adding hydrogen

Hybrid rich- and lean- premixed ammonia-hydrogen combustion for mitigation.., Ukhwa Jin et al, *Combustion and Flame*, 2024

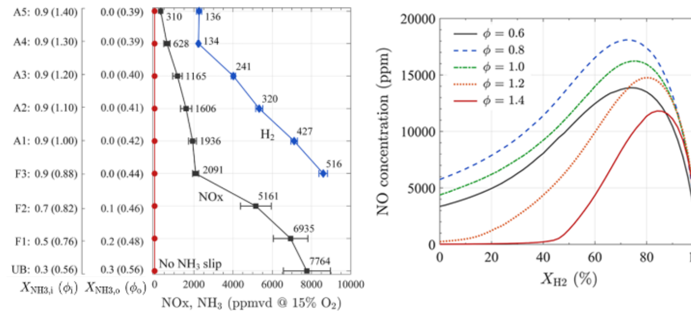
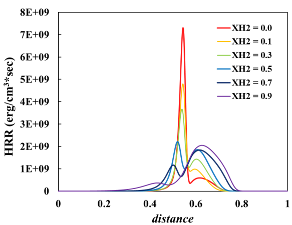
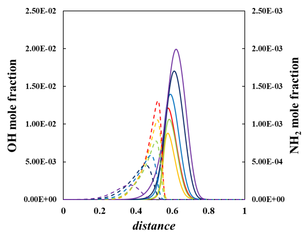


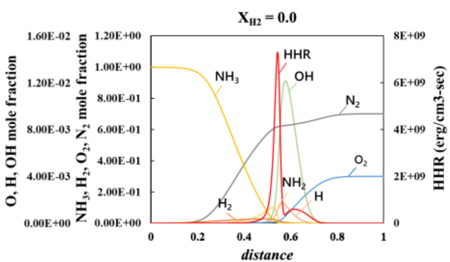
Fig.2 Left Measured total NO_x and unburned NH_3/H_2 emissions, Right Computed NO concentration as a function of NH_3/H_2

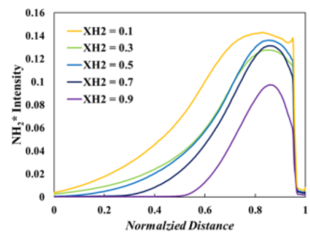
- Adding H_2,
  - Enhances O, H, OH radical formation.
  - Promotes NH_3 decomposition.
  - Stable combustion can be achieved under low O_2.
- At high equivalence ratios,
  - NO initially increases and then decreases .

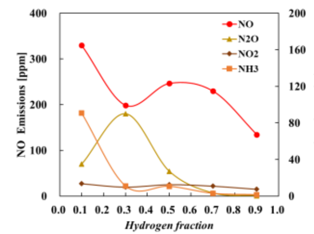
Numerical analysis (CHEMKIN Pro 1-D)	Experimental analysis (laminar diffusion flame)
• Reaction pathway • H, OH, NH_2 Radical behavior • Heat release rate distribution	• Flame images • NH_2* chemiluminescence • Gas emissions (NH_3, NO_X)

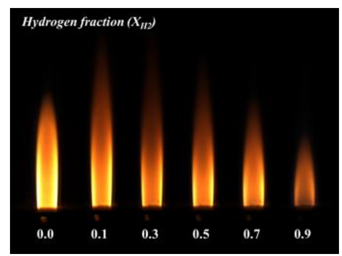






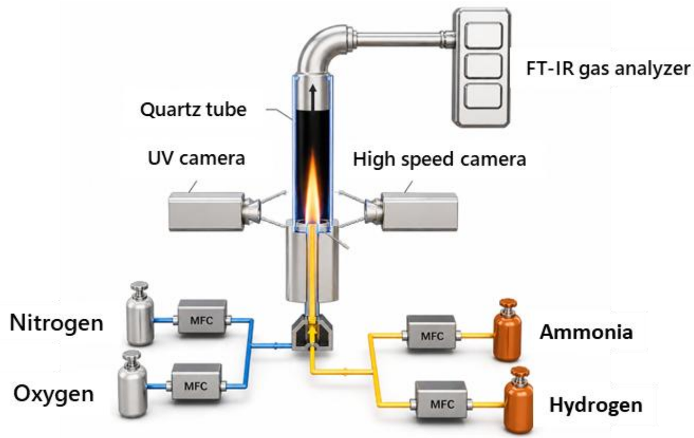






To analysis how H_2 addition modifies flame structure, enhances reaction kinetics and improves the combustion performance of NH_3 fuel.

Schematic of Experimental Apparatus



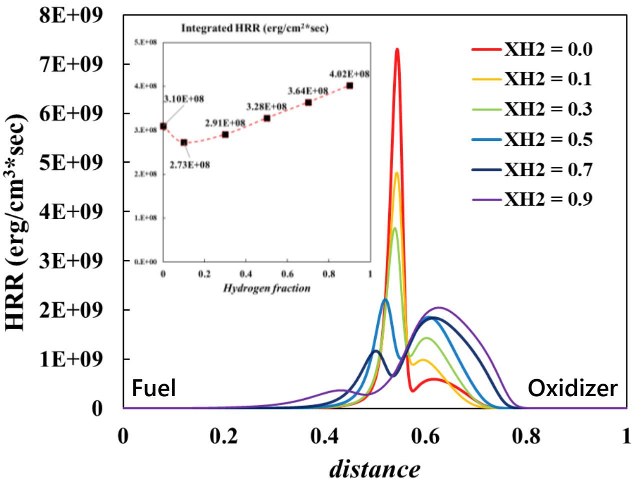
- Experimental setup
  - Fuel inlet (D_o = 10 mm, D_i = 8 mm)
  - Oxidizer inlet (D_o = 25 mm, D_i = 21 mm)
  - FT-IR gas analyzer (Cell e Co., Gasmet Co.)
  - UV-sensitive camera (GO-8105M-5GE-UV)
  - High-speed camera (Fastcam SA4; Photron Co.)
  - Band pass filter : NH_2^* (632 ± 10 nm)

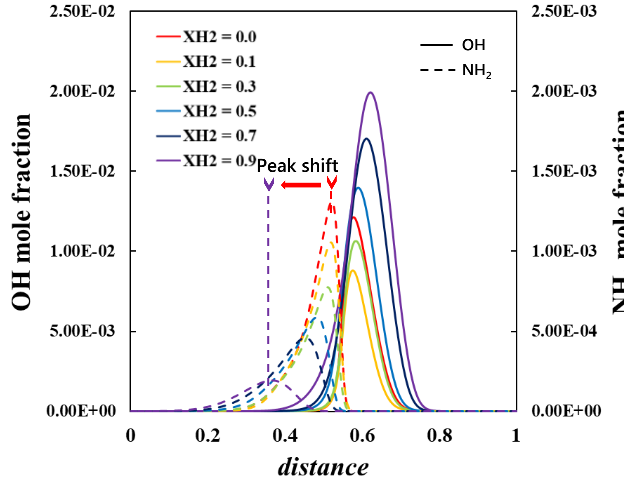
$$* X_{H2} = \frac{x_{H2}}{x_{NH3} + x_{H2}}$$

- Experimental conditions

Num.	X_{H2}	O_2 (%)	Fuel		Oxidizer	
			LPM	Re	LPM	Re
Case1	0.0	30	1	≈ 190	3.57	≈ 251
Case2	0.1	23	1	≈ 170	3.45	≈ 243
Case3	0.3	21	1	≈ 134	3.21	≈ 226
Case4	0.5	21	1	≈ 101	2.98	≈ 209
Case5	0.7	21	1	≈ 70	2.74	≈ 193
case6	0.9	21	1	≈ 40	2.50	≈ 176

Numerical Ammonia & Hydrogen Combustion Characteristics

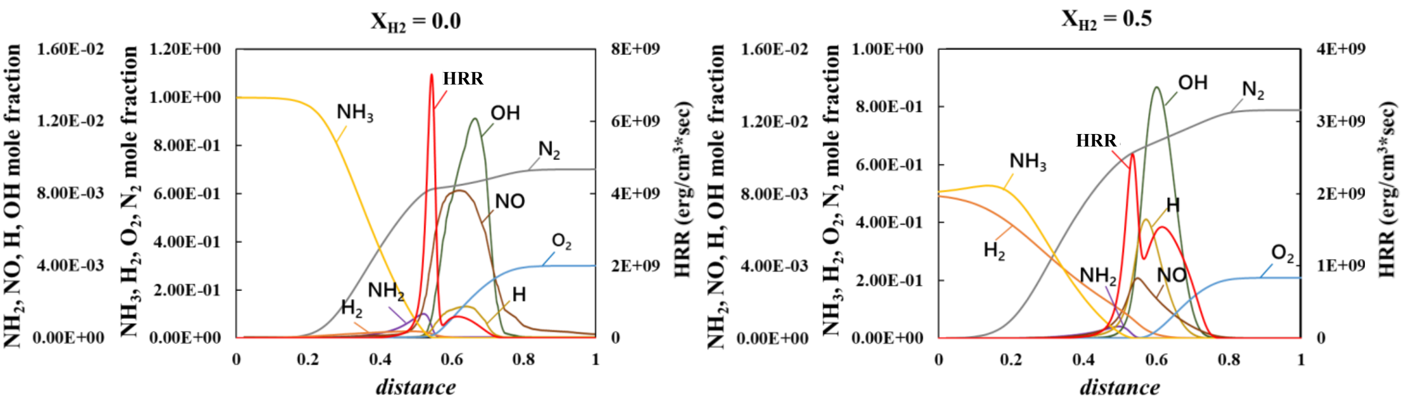




- Heat release rate (HRR) and OH, NH_2 radical profiles

- Pure NH_3 flame shows a sharp and localized peak.
  → high activation E, low reactivity, initial radical pool.
- With H_2 addition, (1)HRR distribution becomes broader, and (2)a dual-peak structure appears.
  → (1)enhances OH radical formation, promotes NH_3 decomposition. (NH_3 -> NH_2 -> NH pathways)
  → (2)The first peak is related to NH_3 decomposition and NH_X oxidation.
  → (2)The second peak is mainly associated with rapid H_2 oxidation.

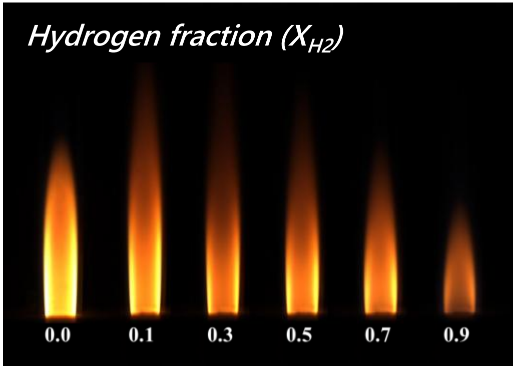
Numerical Ammonia & Hydrogen Combustion Characteristics

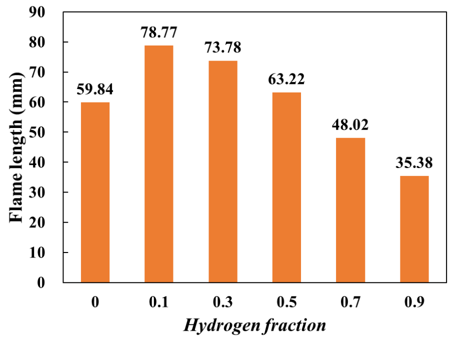


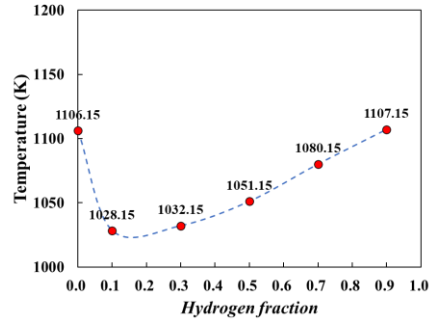
- X_{H2} = 0.0 (NH_3 100%)	- X_{H2} = 0.5
• Single, sharp HRR peak (localized reaction zone)	• Dual HRR peaks (broadened reaction zone)
• Limited H radical pool	• Enhances H, OH radical pool
→ slow reaction initiation	→ promotes NH_3 decomposition
• Higher NO formation	• Lower NO formation
→ dominated by fuel-N pathways	→ reduced fuel-N

➤ Hydrogen addition promotes NH_3 decomposition, broadens the reaction zone, improves flame stability and modifies NO formation.

Direct Flame Images and Flame Temperature







- Flame behavior is influenced by both H_2 addition and O_2 concentration.
- A stable flame for pure NH_3 is achieved only under oxygen-enriched conditions (O_2 30%).
- With H_2 addition :

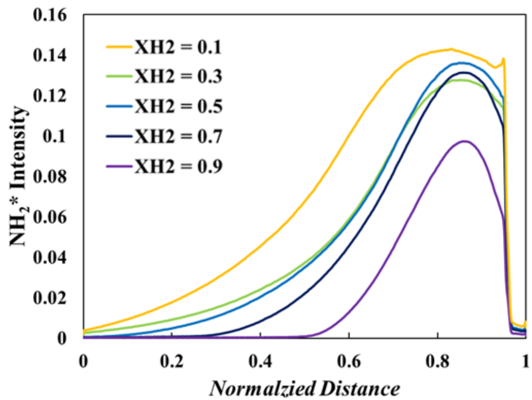
(1)the required O_2 concentration decreases. [O_2 23% (X_{H2} = 0.1), O_2 21% ($X_{H2} \geq 0.2$)]

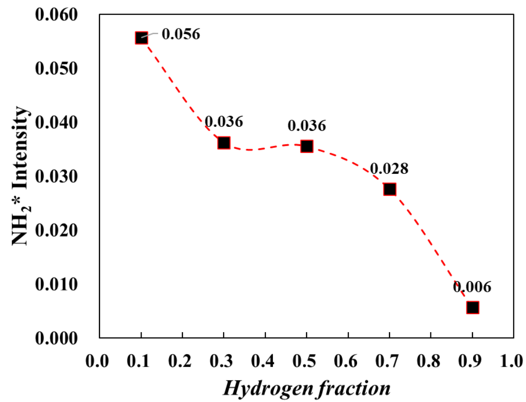
(2)Flame length decreases and flame temperature increases.

→ increases H, OH radical pool.

→ enhances combustion reactivity and faster reaction rates.

Effect of H_2 Addition on NH_2* Chemiluminescence Intensity





- NH_2* intensity is extracted from flames images using 632 ±10nm band-pass filter.
- Effect of H_2 addition :

(1)Overall, NH_2* intensity decreases.

→ reduced NH_3 fuel content.

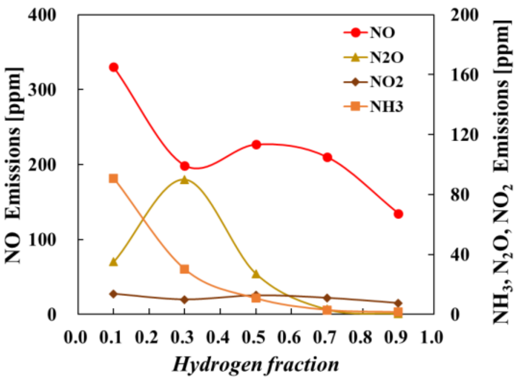
(2)At X_{H2} = 0.3, 0.5, 0.7, NH_2* intensity remains relatively high despite reduced NH_3.

→ H_2 addition enhances H, OH radical pool.

→ This promotes NH_3 decomposition and reaction rates.

→ NH_2 formation is sustained or enhance even with reduced NH_3.

Effect of H_2 Addition on Emission Gas Characteristics



O_2 [%]	X_{H2}	NH_3 (ppm)	NO_X (ppm)	NO (ppm)	N_2O (ppm)	NO_2 (ppm)
23	0.1	90.75	378.72	329.92	35.09	13.70
21	0.3	30.09	298.78	198.69	90.12	9.96
21	0.5	10.74	266.54	226.60	27.26	12.67
21	0.7	3.02	224.26	209.81	3.44	11.01
21	0.9	1.58	142.75	134.63	0.52	7.59

- NH_3 concentration rapidly decreases with increasing H_2 fraction. (90.75 → 1.58 ppm).
  → H_2 addition enhances NH_3 decomposition and oxidation.
- NO_X concentration decreases with increasing H_2 fraction. (378.72 → 142.75 ppm)
- NO decreases overall with increasing H_2 fraction. (329.92 → 134.63 ppm)
  → reduced NH_3 fuel content.
- At X_{H2} = 0.5 condition, NO remains relatively high.
  → (1)promotes NH_3 decomposition.
  → (2)N_2O conversions to NO ($N_2O + O \rightarrow 2NO$)
- N_2O initially increases(X_{H2} = 0.3), then decreases at high H_2 fraction. (35.09 → 0.52 ppm)
  ($N_2O + O \rightarrow 2NO$) or ($N_2O + H \rightarrow N_2 + OH$) or ($N_2O + OH \rightarrow N_2 + HO_2$)

- Numerical and experimental results consistently show H_2 addition significantly improves NH_3 combustion characteristics.

→ Expansion of the reaction zone and transition from localized single-peak HRR structure to a dual-stage reaction structure.

→ Increased H, OH radical formation promotes NH_3 decomposition and accelerates reaction.

→ Flame length decreases and flame temperature increases.

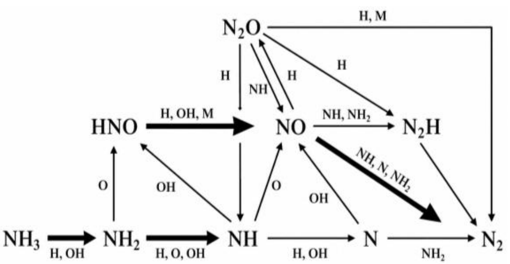
→ Unburned NH_3 decreases and NO_X decreases.

→ N_2O decreases with increasing H_2 fraction (conversion NO or N_2).

$N_2O + O \rightarrow 2NO$

$N_2O + H \rightarrow N_2 + OH$

$N_2O + OH \rightarrow N_2 + HO_2$



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