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Effects of Hydrogen on Ammonia/Methane/Air Combustion in a Can-type Combustor

Zishi Fu[1,2], Wenjin Lai[2,3], Hua Xiao[2]*

[1]Guangzhou Lvzhineng Technology Co., Ltd., Guangzhou 510700, Guangdong Province, China

[2]Guangzhou Maritime University, Guangzhou 510725, Guangdong Province, China

[3]School of Energy and Power Engineering, Chongqing University, Chongqing 400044, China

***Corresponding author:** Hua Xiao, xiaohua.dr@foxmail.com

Abstract: In recent years, the importance of blending traditional methane gas with alternative fuels in combustion to reduce emissions has gained increasing recognition. Existing literature has demonstrated the successful operation of ammonia and hydrogen as fuels in diesel engines. However, there is still insufficient information regarding the combustion of methane in combination with ammonia and hydrogen. This paper investigates the effects of replacing ammonia with hydrogen in blends consisting of 70% CH_4 and 30% NH_3, with hydrogen substitution levels of 0%, 10%, 30%, 50%, 70%, and 90%. The simulation was carried out using the SST k-ω turbulence model and steady diffusion flamelet model. Calculations using Okafor-mech to predict the emission characteristics were also attempted to determine concentration values more accurately. Results show that as the proportion of hydrogen in the blended fuel increases, the maximum temperature rises by 29.28 K. There is an increase in emissions of carbon dioxide and carbon monoxide, while nitrogen oxide emissions decrease.

Keywords: NH3/CH4/H2 combustion; Can combustor; Okafor-mech; Nitrogen oxides; Carbon monoxide

1. Introduction

In recent years, climate change has emerged as a significant issue due to its negative impact on the environment. This has led to an increased focus on green and renewable energy sources. China, facing a growing energy crisis, has set ambitious targets, which are achieving the peak of carbon emissions by 2030 and carbon neutrality by 2060. Energy is the primary source of gas emissions, accounting for about two-thirds [1].

Reducing carbon dioxide emissions is a necessary and primary goal for the development of all nations. This is reflected in the UK's 2050 Net Zero strategy, the United States' rejoining of the Paris Agreement, and China's 2060 Carbon Neutrality targets, all of which emphasize the use of clean energy to reduce carbon emissions [2]. Renewable energies such as wind, solar, and ocean energy have garnered extensive global attention. As of 2021, China's cumulative installed capacity of wind and solar power reached approximately 640 GW, with projections indicating that this capacity will double over the next decade [3]. However, these sustainable energy sources face several barriers and challenges. Due to factors such as weather conditions, seasons, time of day, and regional variations, they are unpredictable and intermittent energy sources. Furthermore, the electricity generated by some of these sources cannot directly connect to the local grid [4]. Consequently, carbon-free fuels offer potential solutions to the challenges posed by these unpredictable and intermittent new energy technologies. Research on the use of ammonia and hydrogen as fuels is gradually gaining public attention [5].

Recent research interest has focused intensely on ammonia (NH_3) combustion due to its potential to mitigate CO_2 emissions in power plants. Combining NH_3 with CH_4 presents a promising solution to this end [6–8]. Despite challenges like low flammability and high NO_x emissions associated with NH_3 fuel, blending it with methane effectively enhances combustibility while maintaining lower carbon emissions [6]. Furthermore, incorporating hydrogen can further reduce the nitrogen content within the fuel, potentially altering NO_x emissions. Research into the combustion characteristics of $NH_3/H_2/CH_4$ mixed fuels lays foundational theoretical support for the broader application of NH_3 blended fuels [7].

Cellek et al. investigated H_2/NH_3 fuel combustion and NO_x emissions under varying ammonia concentrations (5%, 10%, 20%, and 50%) and excess air ratios [8]. They found that reduced NO_x emissions with increasing ammonia enrichment. Gotama et al. studied NH_3/H_2/air flame kinetics under rich fuel and high pressure, measuring burning velocities at equivalence ratios of 0.1 and 0.5 MPa [9]. Han et al. conducted experimental research on NH_3 as a fuel in NH_3/air, NH_3/ H_2/air, NH_3/CO/air, and NH_3/ CH_4/air flames, and found that blending NH_3 with H_2 enhances burning rates [10]. Wang et al. extensively studied the combustion characteristics of ammonia/hydrogen mixtures under different initial conditions, including laminar burning velocities, minimum ignition energy, NO_x and ammonia emissions, and combustion efficiency. Their results demonstrated that under conditions relevant to engines, most properties of ammonia/hydrogen fuels are comparable to hydrocarbon fuels [11]. Syed et al. discovered that in a tangential swirl burner using a ternary blend of ammonia, hydrogen, and methane, the formation of OH*, CH*, and NH* decreased with the increase in ammonia content under high equivalence ratio conditions. At $\Phi = 1.2$, a 20/55/25% (vol) $CH_4/NH_3/H_2$ blend resulted in lower emissions [12]. Hua et al. conducted numerical simulations on the co-combustion of ammonia and methane, revealing that the use of ammonia in the mixture significantly reduced CO emissions. Additionally, numerical simulations of engine-related operating conditions indicated that high pressure could reduce NO and CO emissions [13].

2. Numerical modelling

The study employed a geometric model of the can-type combustor, as illustrated in **Figure 1**. Primary air enters the combustion chamber through the main inlet at the base of the canister. Six swirl inlet vanes guide this incoming air into the canister, mixing it with pure methane to facilitate proper combustion. As the mixture reacts within the canister, secondary air is introduced into the combustion chamber through six secondary air inlets located downstream from the primary combustion zone. This enhances combustion efficiency and helps cool the canister walls exposed to the hot reacting flow. This study investigates the impact of substituting ammonia with hydrogen at levels of 10%, 30%, 50%, 70%, and 90% in the combustion of a blended fuel consisting of 70% methane and 30% ammonia. The simulation is conducted under normal temperature and pressure conditions.

Figure 1. Mesh of the Combustor

SST k-ω turbulence model is chosen, and the steady diffusion flamelet model is applied to $NH_3/H_2/CH_4$/air combustion fields generated by a can combustor. Moreover, Okafor-mech, which is known for its best simulation performance in the numerical simulation of NH_3/CH_4 fuel, was utilized [14]. Additionally, a presumed mixture composition probability density function (PDF) is introduced to characterize the mutual interaction of turbulent combustion reactions.

The importance of co-combusting traditional methane gas with alternative fuels to reduce emissions in combustion has grown in recent years. While the literature confirms the successful use of ammonia and hydrogen as fuels in diesel engines, there remains a lack of adequate information regarding the combustion dynamics when methane is combined with both ammonia and hydrogen. This study aims to numerically investigate the effects of methane-hydrogen and methane-ammonia-hydrogen fuel mixtures on system performance and emissions.

3. Results and discussion

The contours of the temperature field and NO_x when replacing ammonia with hydrogen in blends consisting of 70% methane and 30% ammonia, with hydrogen substitution levels of 0%, 10%, and 90% are shown in **Figure 2a**. The red area in **Figure 2a** becomes a deeper shade of red as the amount of hydrogen injection increases. This is because hydrogen releases more energy, intensifying the combustion process. As observed in **Figure 2b**, there is a significant decrease in the mole fraction of NO as the amount of hydrogen increases. However, in **Figure 2c** and **Figure 2d**, the mole fractions of CO and CO_2 increase with the addition of hydrogen. It is worth noting, though, that the increase in the mole fractions of CO and CO_2 is minimal. The area-weighted average temperature and the highest temperature at the outlet are shown in **Figure 3**. As the hydrogen blend ratio increases from 0% to 27%, the average temperature of the profile decreases from 1156.4 K to 1136.0 K. From the contour plots, the temperature distribution shows insensitivity to variations in the ammonia-to-hydrogen ratio. However, as the H_2 mass fraction increases, the flame temperature slightly rises, resulting in the peak temperature increasing from 2176.5 K to 2205.8 K. This is attributed to the fact that hydrogen releases significantly more energy during combustion compared to ammonia and methane. Under the same conditions, hydrogen can release more heat, and this high energy release results in a more intense combustion process, thereby increasing the flame propagation speed. Moreover, the combustion speed of hydrogen itself is much faster than that of ammonia and methane, further accelerating the spread of the flame within the combustion zone. Consequently, when hydrogen is mixed with ammonia and methane for combustion, the high energy release and rapid combustion characteristics of hydrogen dominate the flame propagation speed, making the entire combustion process more efficient.

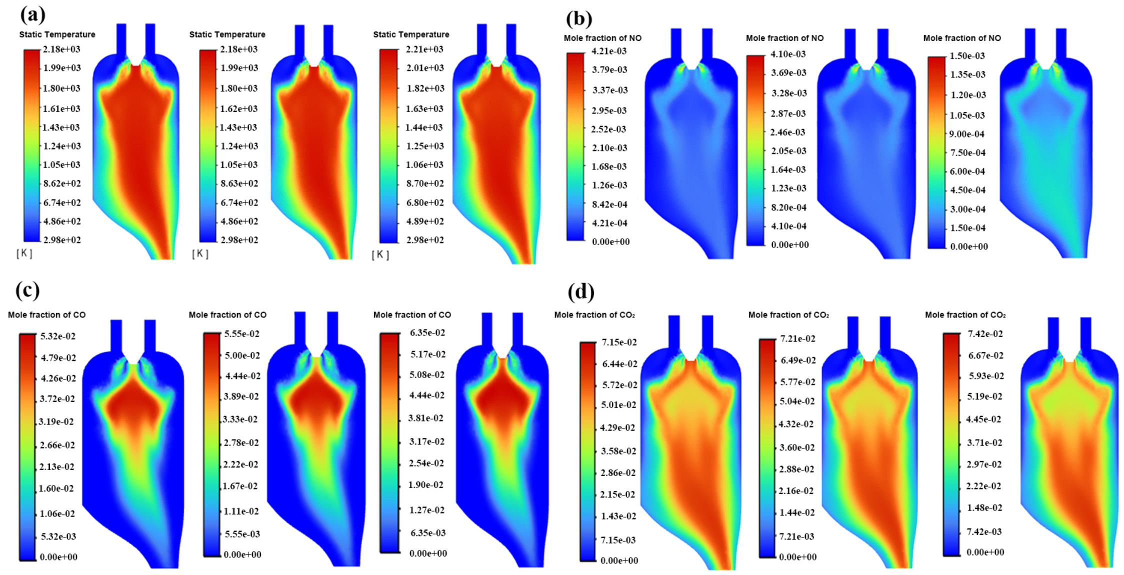

Figure 2. (a) Contours of temperature field in the combustor (left to right: 30%NH_3, 0%H_2, 70%CH_4; 27%NH_3, 3%H_2, 70%CH_4; 3%NH_3, 27%H_2, 70%CH_4). (b) Contours of NO mole fraction in the combustor (left to right: 30%NH_3, 0%H_2, 70%CH_4; 27%NH_3, 3%H_2, 70%CH_4; 3%NH_3, 27%H_2, 70%CH_4). (c) Contours of CO mole fraction in the combustor (left to right: 30%NH_3, 0%H_2, 70%CH_4; 27%NH_3, 3%H_2, 70%CH_4; 3%NH_3, 27%H_2, 70%CH_4). (d) Contours of CO_2 mole fraction in the combustor (left to right: 30%NH_3, 0%H_2, 70%CH_4; 27%NH_3, 3%H_2, 70%CH_4; 3%NH_3, 27%H_2, 70%CH_4).

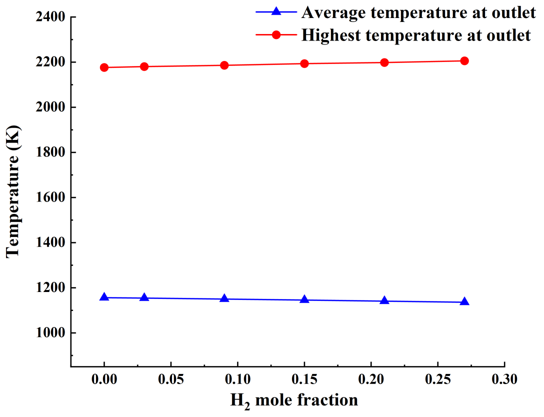

Figure 3. Temperature at outlet against H_2 mole fraction

Figure 4a and **Figure 4b** represent the different levels of CO and CO_2 emissions, respectively, as the hydrogen content in the blend increases. When highly reactive hydrogen is introduced, intense and complex turbulent exchanges occur within the combustion chamber, promoting thorough mixing of the fuel-air mixture and facilitating the conversion of CO into CO_2 through reactions. Unexpectedly, it can be observed that with an increase in hydrogen volume fraction, CO and CO_2 emissions increased overall. Therefore, when NH_3, H_2, and a fixed proportion of CH_4 burn together, increasing the proportion of ammonia is beneficial for reducing CO_2 emissions. Although the mole fractions of CO and CO_2 exhibit an upward trend, their increases are minimal. The mole fraction of CO_2 only increased from 0.0332 to 0.0337, and the mole fraction of CO rose by only 0.0014.

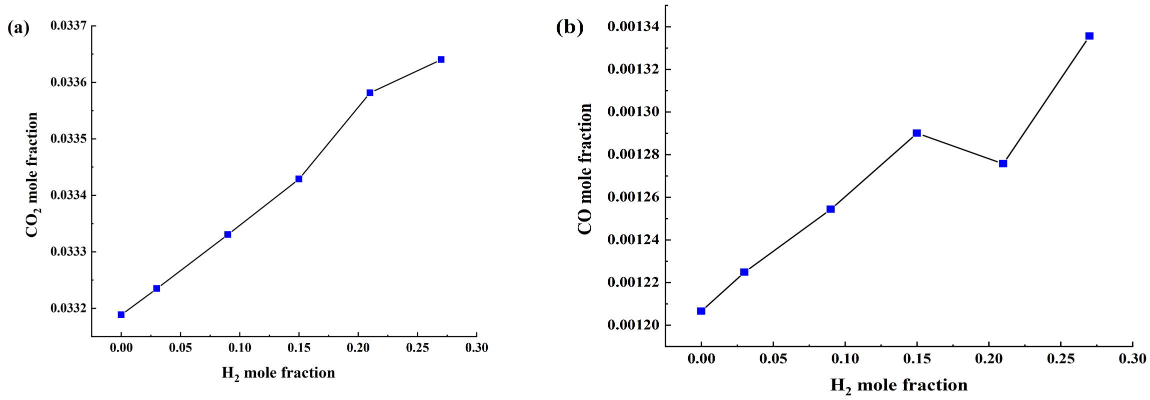

Figure 4. (a) Average CO_2 mole fraction in exhaust against H_2 mole fraction; (b) Average CO mole fraction in exhaust against H_2 mole fraction

According to **Figure 5a**, increasing hydrogen mole fractions in the blend have decreased considerably the NO emission. However, in industrial production, both excess and insufficient oxygen can cause unnecessary complications in the operation of chemical facilities. This variation in oxygen baselines among industries is why directly comparing emission standards based on these different baselines is not feasible. Therefore, all industries' air pollutant emission standards include a provision requiring that measured emission concentrations be converted to baseline oxygen concentrations. For gas turbines, the baseline oxygen content is set at 15%.

Figure 5b shows that the increasing hydrogen fractions in the blend have decreased the NO_x emission. There are three types of NO_x generation: thermal NO_x, fuel NO_x, and transient NO_x. In this case, the impact of transient NO_x is relatively minor and can be disregarded. Adding hydrogen increases the maximum combustion temperature, leading to higher thermal NO_x emissions. Simultaneously, substituting hydrogen for ammonia reduces the nitrogen content in the fuel, thereby decreasing fuel NO_x formation. This substitution effect of hydrogen results in a stronger reduction in NO_x emissions overall.

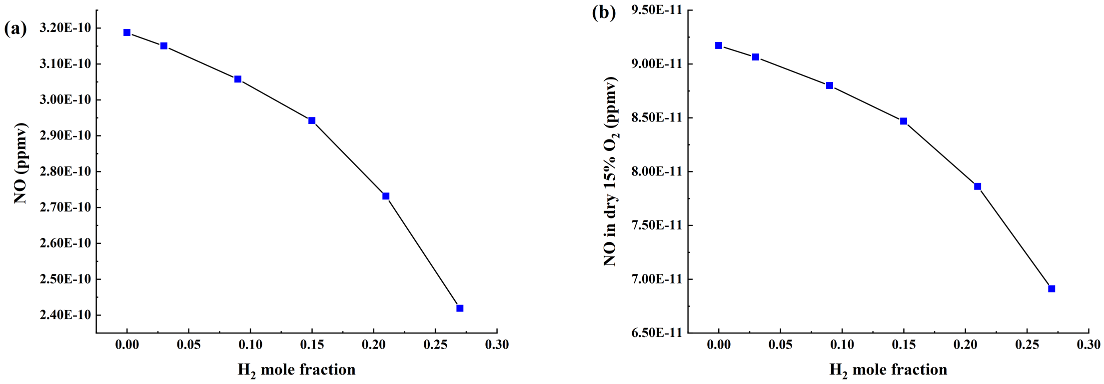

Figure 5. (a) Average NO mole fraction in exhaust against H_2 mole fraction; (b) Normalized (Dry 15% O_2) NO in exhaust against H_2 mole fraction

4. Conclusions

The depletion of fossil fuels and their detrimental impact on climate change have heightened the demand for alternative and renewable energy sources. This has led to increased research in the field. Among the emerging non-fossil fuels, CH_4 and H_2 have gained significant attention due to their advantageous characteristics. Hydrogen, in particular, is highly attractive due to its high calorific value, clean combustion with zero carbon emissions, and favorable combustibility. However, its high flame temperatures and the associated risk of flame flashback necessitate effective strategies to manage elevated NO_x emissions. Simultaneously, NH_3 has also garnered interest as a potential energy carrier and carbon-free combustion fuel. This study aims to investigate the influence of varying hydrogen-ammonia ratios and methane mixtures on combustion characteristics and emissions.

As the hydrogen ratio increased from 0% to 30%, the peak temperature inside the combustion chamber rose from 2176.5 K to 2205.8 K. However, the average temperature at the outlet decreased from 1156.4 K to 1136.0 K. This is attributed to the higher energy release and intensity of hydrogen combustion compared to ammonia and methane, leading to a higher rate of flame propagation.

With the higher hydrogen ratio, there was an overall increase in CO_2 and CO emissions. The introduction of more reactive hydrogen leads to more intense and complex turbulent exchange reactions within the combustion chamber, promoting the thorough mixing of the fuel-air mixture and thereby increasing CO_2 and CO emissions. However, the increases in CO_2 and CO emissions are negligible, amounting to only 0.0005 and 0.0014, respectively. Increasing the hydrogen ratio led to a reduction in NO_x emissions and only slightly increased CO_2 and CO emissions from combustion. While hydrogen addition intensified the production of thermal NO_x, it significantly reduced the competitiveness of fuel NO_x emissions.

Disclosure statement

The authors declare no conflict of interest.

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