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Combustion and Emission Characteristics of Ammonia/Hydrogen dual-fuelled Generic Gas Turbine

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Abstract
To develop a generic gas turbine dual-fuelled by ammonia/hydrogen with high combustion efficiency and low NO_x emission, an in-depth understanding of combustion and emission characteristics of premixed ammonia/hydrogen flame in generic gas turbine is essential. Over a wide range of equivalence ratios, hydrogen blending ratios and oxygen contents in the oxidizer, an appropriate initial component ratio is firstly selected for subsequent parametric study. The influence of pressure, inlet temperature and secondary air injection on peak heat production rate, outlet temperature and emission (NH_3, H_2, NO_x) are investigated. Results show that the outlet temperature is slightly increased with either pressure augmentation or inlet temperature enhancement. The increase in pressure promotes the reduction of NO_x in the post-flame zone, and it has a greater influence on fuel-bound NO than thermal-NO. An increase of NO emission is found as inlet temperature rises due to the extended Zel'dovich mechanism. In addition, the secondary air injection is beneficial to the improvement of combustion efficiency, but since the NO consumption reaction is incomplete and the nitric oxide is oxidized by excess air, a considerable increase in NO and NO_2 emissions is observed. Thus, it is required to choose an appropriate amount of secondary air to balance the high combustion efficiency and low NO_x emission.

Introduction

In response to global warming, many countries are committed to achieving Net Zero target [1]. For example, the UK has enacted a law to reach net-zero greenhouse gas (GHG) emissions by 2050. Accordingly, extensive research has been conducted on renewable and low-carbon based power generation in recent decades. Ammonia (NH_3), as a carbon-free substance and potential hydrogen carrier, is a promising alternative fuel. It can be easily compressed under $8\ bar$ at room temperature or liquified at $-34℃$ under atmospheric pressure, which is similar as propane storage [2-4]. The transportation infrastructure of ammonia is also reliable, with approximately 100 million tons delivered annually [5]. Moreover, the industrial ammonia production is well-existing mainly known as Haber-Bosch process and ammonia can also be obtained using new synthesis technology with sustainable and renewable energy [6, 7].

However, ammonia has a narrow flammability range (around $18\% - 28\%$ fuel mole fraction) [3], high ignition temperature and low flame speed (one-fifth flame speed of methane flames) [8], which makes it difficult to stabilize the ammonia combustion and achieve a high combustion efficiency. Hydrogen is widely introduced as a promoter in ammonia combustion, as hydrogen has a high reactivity and flame speed and it is also a clean fuel and can be produced directly from ammonia decomposition. Han et al. examined premixed laminar burning velocity of NH_3/air, NH_3/H_2/air, NH_3/CO/air and NH_3/CH_4/air with heat flux method [9]. Hydrogen is found to be the most effective additive to increase the burning velocity of ammonia flame. Laminar flame speed of pure ammonia and ammonia/hydrogen premixed flames were measured experimentally at elevated pressure up to $5\ bar$ in Tohoku University [10, 11]. The ammonia premixed flames can reach maximum $7\ cm/s$, while the flame speed increased non-linearly with the increasing hydrogen addition and can achieve more than $100\ cm/s$. Li et al. conducted experiment to investigate NO_x formation and flame speed at various equivalence ratios ($1.00 - 1.25$) and initial hydrogen concentrations ($33.3 - 60.0\%$) in the fuel and also numerically studied the effect of hydrogen addition ($0.0 - 0.5$) on heat release characteristics [4, 12]. The results illustrated that adding hydrogen can improve ammonia combustion behaviour and enhance the heat release rate from both chemical effect and transport effect. Based on the above studies, ammonia/hydrogen blend is considered as a promising alternative fuel for practical power system.

A number of researches on the development of ammonia based power system have been carried out. It was revealed that extensive development such as chemical enrichment by cracking or use of additives and application of multiple combustion chambers is necessary to improve the mixing process efficiency of ammonia-fired gas turbine [13]. Valera-Medina et al. investigated the ammonia/methane flame stability and emissions with a generic tangential swirl gas turbine burner at different equivalence ratios and pressure and results were extended and compared by numerical calculation [14]. It was demonstrated that the total emissions reached lowest at the equivalence ratio between $1.15 - 1.25$, although the level of CO emission was still unacceptable. A different injection strategy and lower swirl number were suggested to optimize the ammonia/methane combustion efficiency. Another generic swirl burner experiment for gas turbine were

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performed with $50\%NH_3\!:\!50\%\,H_2\,(Vol)$ at the premixed fuel-lean conditions under normal temperature and pressure, finding the flame was stable at a narrow equivalence ratio $(0.43-0.52)$ and NO_x emission were higher than that under fuel-rich conditions [15]. Hussein et al. simulated a new injection strategy in a swirl burner to further reduce NO_x emission from ammonia/hydrogen combustion [16]. As a result, as more ammonia/hydrogen was injected downstream of the primary flame zone, the level of NO formation decreased. Moreover, NO emission was further reduced with the increase of residence time in the second recirculation zone. National Institute of Advanced Industrial Science and Technology (AIST) in Japan succeeded in implementing $50\,kW$-class micro gas turbine power generation fuelled by ammonia/kerosene [17] and ammonia [8]. Regenerator and diffusion combustion were used to keep ammonia combustion robust. SCR (Selective Catalytic Reduction) technology was used to reduce NO_x, but the SCR equipment was large in scale, which was recognized to be the weakness of the system. Therefore, for the purpose of developing a low-NO_x high-efficiency combustor in generic gas turbine fuelled by ammonia/hydrogen, initial component ratios, working conditions and injection strategies are necessary to be further studied.

This paper investigates combustion and emission characteristics of premixed ammonia/hydrogen flame in a generic gas turbine. First of all, an appropriate initial component ratio combination is determined over a wide range of equivalence ratios, hydrogen blending ratios, oxygen contents in the oxidizer. Then, based on the determined initial component ratios, the effects of pressure, inlet temperature and secondary air injection on heat production rate, outlet temperature and emissions are studied to improve the combustion efficiency and minimize NO_x emission.

Methodology

In this work, combustion and emission characteristics of ammonia/hydrogen dual-fuelled generic gas turbine are numerically calculated with Ansys Chemkin Pro based on Nakamura's detailed ammonia reaction kinetic mechanism [18] which has been validated in the previous work [19]. The sub-model in Chemkin Pro, gas turbine network, is utilised to predict the peak heat reaction rate, outlet temperature and emissions (NH_3, H_2, NO_x). The gas turbine network contains three Perfectly Stirred Reactors (PSRs) which represent mixing zone, recirculation zone and flame zone respectively, and a Plug Flow Reactor (PFR) which represents post-flame zone. It is commonly employed to calculate mixing and flow characteristics of a gas turbine combustor [20]. Two different system schematics are shown in Figure 1. The premixed fuel (ammonia and hydrogen) and oxidizer (oxygen and nitrogen) are injected into the mixing zone, and then passed through the recirculation zone and delivered to the flame zone. The system is used to analyse the effects of initial component ratios and working conditions. To study the injection strategy, secondary air is introduced and injected into the flame zone, which is

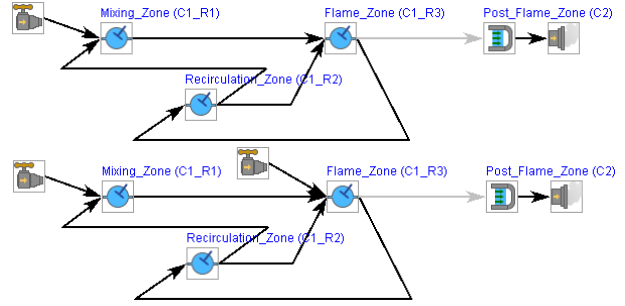expected to improve the combustion efficiency (reduce the unburnt fuel).

Figure 1. System schematics.

Thus, initial component ratios, for example, fuel-air equivalence ratio (ϕ), hydrogen blending ratio (mole fraction of hydrogen in the fuel, $x\%H_2$) and oxygen content in the oxidizer (mole fraction of oxygen in the oxidizer, Ω), working conditions (pressure (P_1) and inlet temperature (T_1)) and injection strategy (secondary air injection) are critical parameters to avoid high emissions and improve combustion efficiency. Table 1-6 illustrate the initial conditions for each case and range for various parameters. The initial component ratios will be selected based on the results of first three tables for further parametric analysis on working conditions and injection strategy. The mass flow rate of inlet ammonia keeps constant at $0.851\,g/s$ in all cases. The recirculation is set as 20% of the product gases [15]. According to the test rig to be used for data validation, the diameter and length of the duct are set as $150\,mm$ and $300\,mm$, respectively.

Table 1. Initial conditions for investigating the effect of equivalence ratio ($T_1 = 300\,K, P_1 = 1\,bar, \dot{m}(NH_3) = 0.851\text{g/s}$).

ϕ	$x\%H_2$	Ω	$\dot{m}(H_2)$ (g/s)	$\dot{m}\,(O_2)$ (g/s)	$\dot{m}(N_2)$ (g/s)
0.8				1.752	5.767
0.9				1.557	5.126
1	0.2	0.21	0.025	1.402	4.614
1.1				1.274	4.194
1.2				1.168	3.845

Table 2. Initial conditions for investigating the effect of hydrogen blending ratio ($T_1 = 300\,K, P_1 = 1\,bar, \phi = 1.1, \Omega = 0.21, \dot{m}(NH_3) = 0.851\text{g/s}$).

ϕ	$x\%H_2$	Ω	$\dot{m}(H_2)$ (g/s)	$\dot{m}\,(O_2)$ (g/s)	$\dot{m}(N_2)$ (g/s)
	0		0.000	1.092	3.595
	0.1		0.011	1.173	3.861
1.1	0.2	0.21	0.025	1.274	4.194
	0.3		0.043	1.404	4.622
	0.4		0.067	1.578	5.193

Table 3. Initial conditions for investigating the effect of oxygen content in the oxidizer ($T_1 = 300\ K, P_1 = 1\ bar, \dot{m}(NH_3) = 0.851$ g/s).

ϕ	$x\%H_2$	Ω	$\dot{m}(H_2)$ (g/s)	$\dot{m}(O_2)$ (g/s)	$\dot{m}(N_2)$ (g/s)
		0.21			5.193
		0.4			2.071
1.1	0.4	0.6	0.067	1.578	0.920
		0.8			0.345
		1			0.000

Table 4. Initial conditions for investigating the effect of initial pressure ($\phi = 1.1, x\%H_2 = 0.4, \Omega = 0.4, \dot{m}(NH_3) = 0.851$ g/s, $\dot{m}(H_2) = 0.067$ g/s, $\dot{m}(O_2) = 1.578$ g/s, $\dot{m}(N_2) = 2.071$ g/s).

$T_1\ (K)$	$P_1\ (bar)$
	1
	5
300	10
	15
	20

Table 5. Initial conditions for investigating the effect of initial temperature ($\phi = 1.1, x\%H_2 = 0.4, \Omega = 0.4, \dot{m}(NH_3) = 0.851$ g/s, $\dot{m}(H_2) = 0.067$ g/s, $\dot{m}(O_2) = 1.578$ g/s, $\dot{m}(N_2) = 2.071$ g/s).

$T_1\ (K)$	$P_1\ (bar)$
300	
350	
400	1
450	
500	

Table 6. Initial conditions for investigating the effect of secondary air injection under standard temperature and pressure (Primary injection: $\phi = 1.1, x\%H_2 = 0.4, \Omega = 0.4, \dot{m}(NH_3) = 0.851$ g/s, $\dot{m}(H_2) = 0.067$ g/s, $\dot{m}(O_2) = 1.578$ g/s, $\dot{m}(N_2) = 2.071$ g/s).

Secondary air injection	
$\dot{m}\ (Air)(g/s)$	$\phi_{overall}$
0.100	0.973
0.500	0.877
1.000	0.780
3.000	0.542
7.000	0.337

Results and discussion

The influence of equivalence ratio at $0.8 - 1.2$ on peak heat production rate, outlet temperature and emissions are discussed in Figure 2. It illustrates the peak heat production rate of ammonia/hydrogen combustion in gas turbine rises with the increasing equivalence ratio under fuel-lean conditions, reaches the peak at the stoichiometric condition and decreases under fuel-rich conditions. It can also be observed the same trend in the outlet temperature. It is because the equivalence ratio determinates the inlet flame speed, which has a direct effect on the heat production rate. Flame speed of ammonia/hydrogen is increased as equivalence ratio increases and peaks at around the equivalence ratio of unity before it decreases at fuel-rich conditions. Figure 2(b) shows that NO_x emission decreases with the increase of equivalence ratio, but the unburnt ammonia and hydrogen rises. Although thermal-NO has a greater influence on both NO production and consumption with a higher equivalence ratio, the significant increase in NO consumption via NH_i and N contributes to the decreased NO formation. However, as a large amount of unburnt ammonia and hydrogen would reduce the combustion efficiency, extremely high equivalence ratio is not recommended. Considering NO_x emission at fuel-lean conditions is much higher than that in fuel-rich conditions, an equivalence ratio at 1.1 is suggested for further investigation. Meanwhile, the heat production rate and outlet temperature at the equivalence ratio of 1.1 are also at a high level.
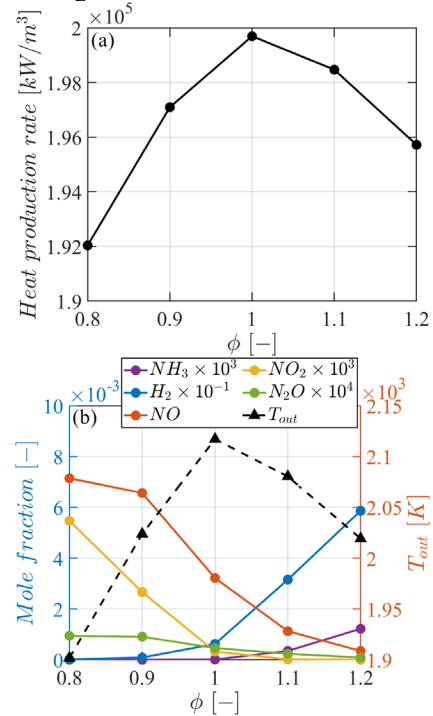

Figure 2. Influence of equivalence ratio on (a) peak heat production rate, (b) outlet temperature and emissions.

Hydrogen enrichment and oxygen enrichment are two effective methods to enhance the flame speed of ammonia flames and adiabatic temperature to stabilize ammonia combustion. Figure 3 and 4 reveal the influence of hydrogen blending ratio up to 0.4 and oxygen content in the oxidizer from 0.21 to 1.00 on ammonia/hydrogen combustion and emission characteristics in a generic gas turbine. It can be seen that the peak heat production rate and outlet temperature are both increased as more hydrogen is introduced into the fuel or oxygen content is increased in the oxidizer due to the increase of the flame speed. As shown in Figure 3, since hydrogen has a very
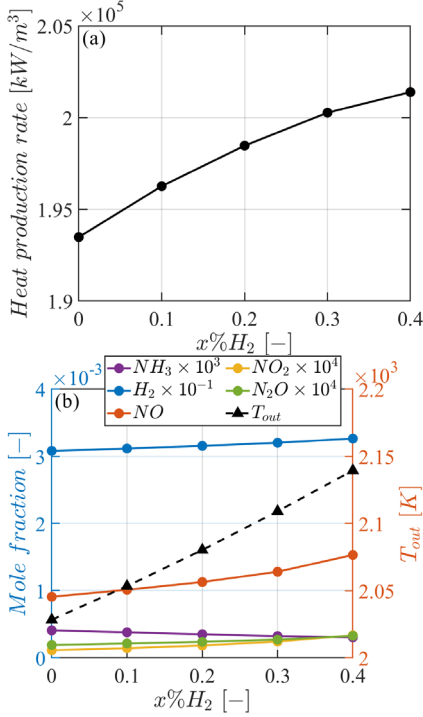
Figure 3. Influence of hydrogen blending ratio on (a) peak heat production rate, (b) outlet temperature and emissions.
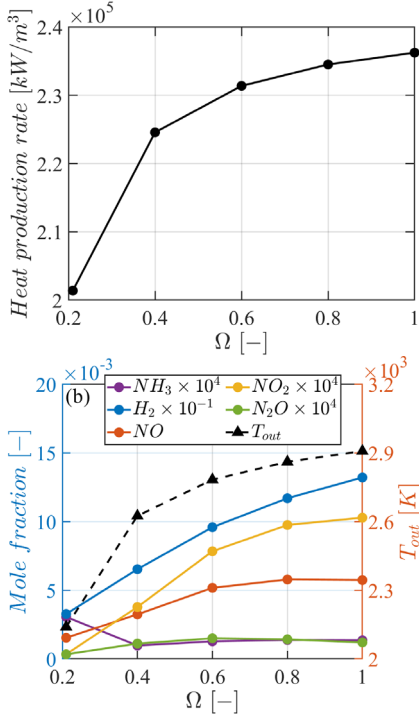

Figure 4. Influence of oxygen content in the oxidizer on (a) peak heat production rate, (b) outlet temperature and emissions.

high reactivity, the heat production rate is promoted to a much higher level with 40% hydrogen addition while the outlet temperature has an almost linear relationship with the increase in hydrogen concentration. Figure 4 demonstrates that enriched-oxygen environment significantly enhances the peak heat production rate and

outlet temperature, in particular when the oxygen content in the oxidizer is in the range of $0.21 - 0.4$. Figure 3(b) also shows that NO_x emission slightly increases when more hydrogen is blended with ammonia. The temperature is improved effectively with a higher hydrogen blending ratio. In a higher temperature environment, thermal-NO_x are dominate in both NO_x formation and consumption, but the rate of NO_x production is higher than the rate of NO_x consumption. Therefore, it leads to the increasing trend in NO_x emission. Considering the robustness of the flame, although adding hydrogen causes more NO_x emission, it is recommended to set the hydrogen blending ratio to 0.4. The laminar flame speed of $40\%H_2/60\%NH_3$ ($\phi = 1.1$) is similar to that of methane flames at the same working conditions [19]. The emission characteristics are illustrated with various oxygen contents in the oxidizer in Figure 4(b). The maximum unburnt ammonia reaches when air is employed as oxidizer ($\Omega = 0.21$). It considerably decreases as the oxygen content rises to 0.4 in the oxidizer and slightly increases as oxygen content is over 0.4. The reason of this phenomena is that ammonia combustion is incomplete when oxygen content is 21% in the oxidizer. More oxygen contents promote the ammonia flame speed which leads to complete ammonia oxidation. In addition, it is also found that oxygen enrichment results in the increase of unburnt hydrogen and NO_x emission. In order to complete the combustion of ammonia and hydrogen and minimize other gas emissions, the oxygen content at 0.4 in the oxidizer is chosen to employ for subsequent analysis.
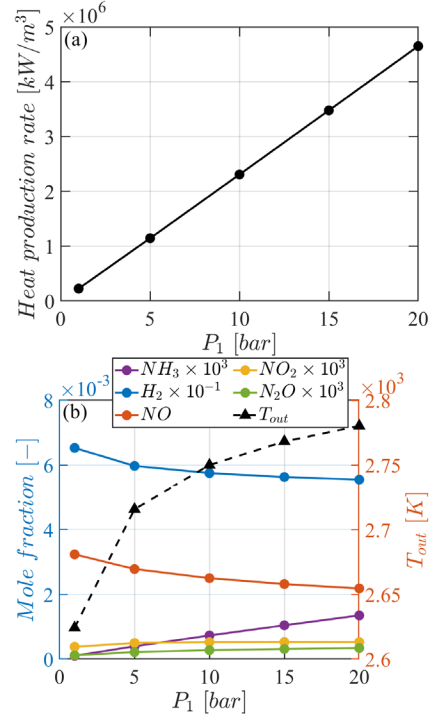

Figure 5. Influence of pressure on (a) peak heat production rate, (b) outlet temperature and emissions.

Figure 5 and 6 demonstrate the influence of pressure ($1 - 20\ bar$) and inlet temperature ($300 - 500\ K$) at

the chosen initial component ratios ($\phi = 1.1$, $x\%H_2 = 0.4, \Omega = 0.4$). As shown in Figure 5, as the pressure increases, the peak heat production rate increases significantly, while the outlet temperature slightly increases from 2624 to 2780 K. As pressure augments, NH_i oxidation is replaced by NH_i combination reaction, producing N_2 instead of NO [2]. Consequently, it is illustrated in Figure 5(b) that NO_x formation is reduced as the increasing pressure. Although the improved outlet temperature implies the small increase in NO formation via thermal-NO, overall NO emission is lessened. It indicates that pressure has a greater impact on fuel-bound NO than thermal-NO. In real industrial working conditions, high-pressure is beneficial for NO reduction.
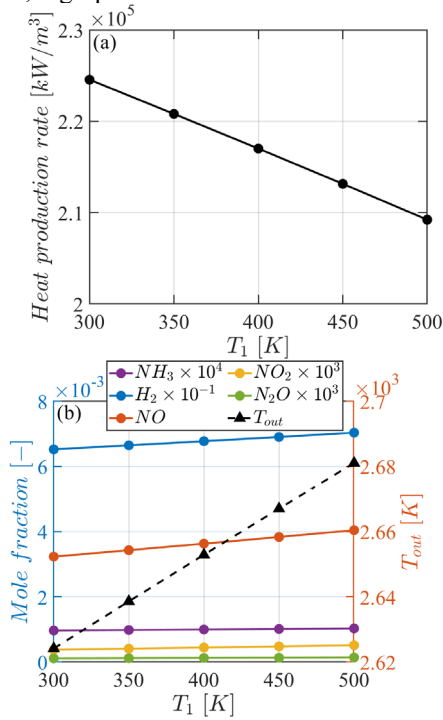

Figure 6. Influence of inlet temperature on (a) peak heat production rate, (b) outlet temperature and emissions.

The peak heat production rate, outlet temperature and emissions with the inlet temperature improvement are plotted in Figure 6. The pressure keeps constant as $1\ bar$. With the increasing of inlet temperature, the outlet temperature increases slightly from $2624\ K$ to $2681\ K$, while the peak heat production rate decreases from 2.25×10^5 to $2.09 \times 10^5\ kW/m^3$. As the initial temperature rises, O/H radical is promoted by extended Zel'dovich mechanism, resulting in high NO concentration in the post-flame zone. It also shows that the unburnt hydrogen is increased while NH_3, N_2O, NO_2 emissions remain unaltered.

Injecting secondary air is commonly utilised to consume unburnt fuel in order to improve the combustion efficiency. When maintaining the primary equivalence constant as 1.1, secondary air injection is employed in the flame zone from 0.100 to 7.000 g/s. The overall equivalence ratio, therefore, is decreased from 0.973 to 0.337. Figure 7 depicts the peak heat production rate, outlet temperature and emissions as a function of overall
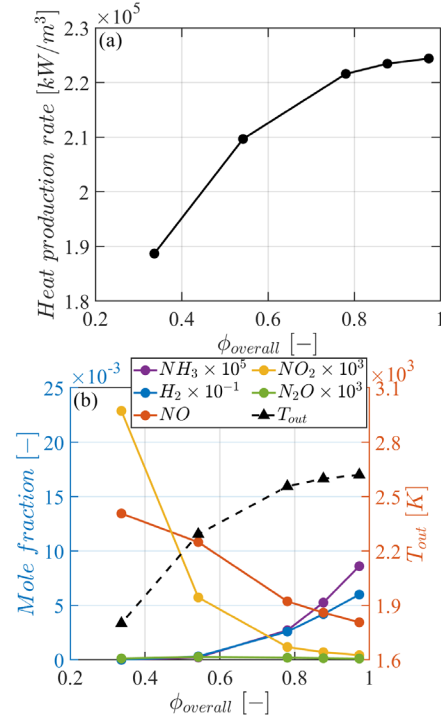

Figure 7. Influence of secondary air injection on (a) peak heat production rate, (b) outlet temperature and emissions.

equivalence ratio. Both peak heat production rate and outlet temperature rises with increase in the overall equivalence ratio, which indicates injecting more secondary air would decrease the heat production rate and outlet temperature. In Figure 7(b), although the unburnt ammonia and hydrogen is lessened with more secondary air injection, NO and NO_2 emissions increase considerably. The secondary air injection reduces the flame speed, resulting in the NO consumption reactions have yet fully proceeded. Additionally, a large amount of NO reacts with oxygen in the secondary air, producing a lot of NO_2 emission in the post-flame zone. It reflects that a large amount of secondary air injection is not the best way to reduce NO_x emission. There is a need to maintain a good balance between high combustion efficiency and low NO_x emission.

Conclusions

In this work, combustion and emission characteristics of premixed ammonia/hydrogen flame in a generic gas turbine are studied with gas turbine network in Ansys Chemkin Pro. An appropriate initial component ratio with 40% hydrogen addition, 40% oxygen in the oxidizer at the equivalence ratio of 1.1 is firstly selected for subsequent parametric study on working conditions and injection strategy. To optimize the combustion efficiency and minimize NO_x emission, the influence of pressure, inlet temperature and secondary air injection on peak heat production rate, outlet temperature and emission (NH_3, H_2, NO_x) are investigated. The major conclusions are summarised as follows. (This work will be validated with additional experiment to extend the knowledge.)

- A slightly increase of outlet temperature and decrease of NO_x formation are found with pressure augmentation. Thermal-NO is promoted as the outlet temperature increases, but the overall NO decreases, implying pressure has a greater influence on fuel-bound NO (compared with thermal-NO) and high-pressure environment is favourable for ammonia/hydrogen dual-fuelled low-NO_x gas turbine.

- With the enhancement of inlet temperature, there is a little increase of outlet temperature. However, O/H radical is increased due to the extended Zel'dovich mechanism, leading to an increase of NO emission.

- For the system with secondary air injection, although combustion efficiency is improved as unburnt fuel are consumed with excess air, NO and NO_2 emissions increase considerably. The slow flame speed caused by secondary air injection leads to incomplete NO consumption reaction and NO oxidation. Thus, it is required to choose an appropriate amount of secondary air to balance the high combustion efficiency and low NO_x emission.

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