

Combustion characteristic of swirl flames using online cracking of ammonia to replace methane in a model gas turbine

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Abstract: As a carbon-free fuel, ammonia has attracted significant attention. However, its low reactivity challenges its application in the realistic combustion system. It is a feasible strategy to enhance ammonia flame using online cracking since the cracked hydrogen could increase the stability, making it more similar to methane flame to realize the replacement. The present work investigates the partially cracked NH₃/air flame in a model gas turbine. Experiment and the large eddy simulation coupled with flamelet generated manifold (FGM) model are conducted. Three NH₃/air cracking ratio cases (cracking ratio, Cr = 0.2, 0.4, 0.6) are investigated. The CH₄ flame under a similar power value condition is also studied for comparison. The results indicate that when the ammonia cracking ratio reaches 40%, the flame structure and heat release characteristics are similar to pure methane flame, but the NO emission increases in cracking cases. (142 words)

Keywords: Ammonia combustion, Partial cracking, Large eddy simulation, Preferential diffusion effect

1. Introduction

Renewable energy, such as wind and solar power, has considerably developed in the past few years. However, questions about these power generation gradually appear. There is an amount of energy loss caused by energy fluctuation. Energy storage is an efficient way to solve it [1]. As we know, hydrogen is a widely acceptable carbon-free fuel containing 120 MJ/kg on a mass basis [2]. Even though some industries put forward the technique routine of hydrogen gas turbines, it is still some distance away from using pure hydrogen fuel in gas turbines widely. Specific to the gas turbine combustor, the biggest challenge is combustion instability, such as flashback and thermal acoustic oscillation. In addition, the high activity properties of hydrogen also led to expensive energy storage and transportation costs. Ammonia is one of the suitable hydrogen carrier fuels, which contains about 17.6% hydrogen in a mass fraction [3]. However, ammonia combustion has two main challenges, i.e., high emission and low combustion stability. Several research groups devote themselves to solving these deficiencies [4-8].

The current research to enhance ammonia combustion mainly focuses on active fuel blending co-firing, such as methane blending and hydrogen blending combustion. However, this strategy doesn't realize the absolute zero-carbon or needs additional fuel, leading to extra costs. Badakhsh et al. [9] pointed out the feasibility of ammonia cracking combustion. The essence of ammonia cracking combustion is increasing enthalpy combustion, which means the process of cracking will add the fuel enthalpy.

Mei et al. [10] studied the laminar flame propagation and kinetic model of NH₃/H₂/N₂/air mixtures. Their research indicates that partial fuel cracking strategies will enhance the combustion intensity. In the cracking fuel strategy, the chemical effect is significant for the enhanced laminar flame propagation, and the reaction H + O₂ (+M) = HO₂ (+M) plays an essential part. The result also reveals that NO formation is a dramatic non-monotonic behavior as the cracking ratio varies. Weseman et al. [11] investigated the blow-out limits of NH₃/H₂/N₂/air flame through experiment and DNS. And the component of H₂ and N₂ follows the “fuel cracking strategies,” i.e., X_{H2}:X_{N2} = 3:1. The blow-out limit of NH₃/H₂/N₂/air flame is compared with CH₄/Air flame under the condition of the similar fundamental parameter. The result shows that the un-stretched laminar flame speed and thermal thickness keep identical because of fast hydrogen diffusion, and the blow-out velocity of NH₃/H₂/N₂/air flame is higher than CH₄/air flame. Bioche et al. [12] studied the NH₃/H₂/air premixed turbulent combustion in a gas turbine swirled burner and found the optimized trade-off equivalence ratio for the such flame. The result shows that the NH₃/H₂/air flame can reach the same power level of the methane flame.

Several research groups have successively studied ammonia cracking combustion since 2019 [10, 11, 13, 14]. However, lots of work are devoted to burning velocity prediction or fundamental investigation. And the research related to NH₃/H₂/air swirl flame didn't consider the ammonia cracking condition. There is nearly no similar research on partial ammonia cracking combustion based on the model gas turbine, according to the best of our knowledge.

This work mainly focuses on the alternative possibility of methane using online partial cracking based on a 20kW model gas turbine. The paper will be separated into three parts. Firstly, the burner and methods will be described. Then, the flame characteristics of methane target flame and ammonia cracking cases will be studied experimentally. To investigate more detailed evidence for replacement, the 1-D simulation and large eddy simulation (LES) will be carried out. Unlike simulation on the methane or ammonia combustion, the non-uniform Lewis number of species must be considered in cracking cases because of the preferential diffusion effect of hydrogen. So the non-uniform Lewis number solver will be used. At last, the heat release characteristic will be investigated by LES.

2. Target flame, cracking flames and research methods

2.1. Brief introduction of total technique routine of ammonia cracking combustion

The source of ammonia comes from chemical factories and electricity-based molecular hydrogen, which is generated from renewable energy. Then ammonia will be directly used for combustion, storage, or distribution. As for the direct use of ammonia, in this routine, the ammonia is cracked partially into hydrogen and nitrogen in advance. Then the cracking fuel, which contains ammonia, hydrogen, and nitrogen, will be used in the gas turbine. In this way, the combustor of GT doesn't need any changes because the fuel characteristic of cracking fuel will be similar to methane. In addition, there is no need to prepare an extra tank to hold another blending fuel, such as methane or other activity fuel.

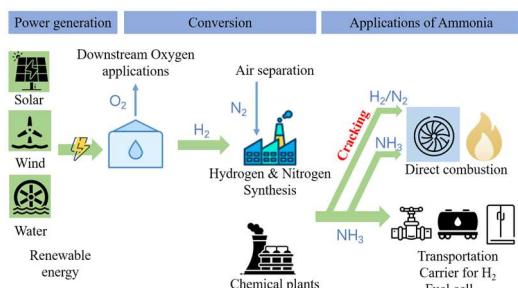


Figure 1 Routine of ammonia cracking combustion

2.2. The Combustor and experimental devices

The target configuration is the 20kW model gas turbine combustor, shown in Fig. 2. It includes a premixing section, a swirller (with 12 vanes and 45° vane angle), and a quartz liner (70×70×180mm). The combustor is operated at ambient conditions (P = 1 atm, T = 300 K). NH₃/H₂/N₂/air will be fully premixed by a mixing chamber in upstream. To ensure the same power, the fuel volume flow rate is 32.9L/min for CH₄ and 83 L/min for NH₃ cases, respectively. We use Nikon D800 for Digital images, OH-PLIF for flame structure, and FTIR for emission, and temperature couple for wall temperature. A detailed introduction of combustor and equipment can be found in our previous research [15].



Figure 2 20 kW model combustor

2.3. Preferential diffusion flamelet generated manifold (FGM) method for CH₄ flame and NH₃/H₂/N₂/air flames

A non-adiabatic FGM method with two control variables (cv) is used in the current study. The FGM table is built by Chem1D [6]. The progress variable is represented by describing the variation from fresh mixture to burnt gas. The other cv is enthalpy, represented by h . In the current study, methane flame is defined as:

$$\gamma = \frac{Y_{C_2O}}{M_{C_2O}} + \frac{Y_{H_2O}}{M_{H_2O}}$$

In ammonia flame, γ is defined as:

$$\gamma = \frac{Y_{H_2O}}{M_{H_2O}} + \frac{Y_{H_2O}}{M_{H_2O}} - \frac{Y_{H_2}}{M_{H_2}} - \frac{Y_{NH_3}}{M_{NH_3}}$$

Where Y_i is the mass fraction of species i , M_i is molecular mass. The definition refers to Donini et al. [16], also certified in our previous study [6]. Conservation equations of continuity and momentum are widely introduced in most simulation research [17]. Besides these equations, the transport equations of progress variable, γ and enthalpy, h are solved in the FGM method. The filtered equations are shown in the following:

$$\begin{aligned} \frac{\partial(\hat{\rho}\tilde{\gamma})}{\partial t} + \nabla \cdot (\hat{\rho}\tilde{\mathbf{u}}\tilde{\gamma}) - \nabla \cdot \left(\left[\left(\widehat{\frac{\lambda}{c_p}} \right) + \frac{\mu_t}{Sc_t} \right] \nabla \tilde{\gamma} \right) &= \nabla \cdot (\hat{d}_\gamma \nabla \tilde{\gamma}) + \hat{\omega}_\gamma \\ \frac{\partial(\hat{\rho}\tilde{h})}{\partial t} + \nabla \cdot (\hat{\rho}\tilde{\mathbf{u}}\tilde{h}) - \nabla \cdot \left(\left[\left(\widehat{\frac{\lambda}{c_p}} \right) + \frac{\mu_t}{Pr_t} \right] \nabla \tilde{h} \right) &= \nabla \cdot (\hat{d}_h \nabla \tilde{\gamma}) \end{aligned}$$

Where ρ is the density, λ is the heat conductivity, c_p is the specific heat capacity of the mixture, and d is the preferential diffusion coefficient introduced later.

In addition, to calculate the NO emission of ammonia flame more correctly [6], the additional transport equation of NO species is also solved:

$$\frac{\partial(\hat{\rho}\tilde{Y}_{NO})}{\partial t} + \nabla \cdot (\hat{\rho}\tilde{\mathbf{u}}\tilde{Y}_{NO}) - \nabla \cdot \left(\left[\left(\widehat{\frac{\lambda}{c_p}} \right) + \frac{\mu_t}{Sc_t} \right] \nabla \tilde{Y}_{NO} \right) = \hat{\omega}_{NO}$$

Where $\hat{\omega}_{NO}$ is the source term of NO. And there is no preferential diffusion term for NO species.

Hydrogen is one of the highly diffusive fuels [18]. So, the preferential diffusion effects cannot be ignored in NH₃/H₂/N₂/air flame calculation, especially in the high hydrogen blending ratio cases. The assumption is that Y_i is related to h and γ , i.e. $Y_i = Y_i(\gamma, h)$. Therefore, the diffusion coefficients can be calculated by [19]:

$$\begin{aligned} d_\gamma &= \frac{\lambda}{c_p} \sum_{i=1}^{Ns} \left(\frac{1}{Le_i} - 1 \right) \alpha_i \left(\frac{\partial Y_i}{\partial \gamma} + \frac{\partial Y_i}{\partial h} \frac{\partial h^{1D}}{\partial \gamma} \right) \\ d_h &= \frac{\lambda}{c_p} \sum_{i=1}^{Ns} \left(\frac{1}{Le_i} - 1 \right) h_i \left(\frac{\partial Y_i}{\partial \gamma} + \frac{\partial Y_i}{\partial h} \frac{\partial h^{1D}}{\partial \gamma} \right) \end{aligned}$$

Where the Le_i is the Lewis number of species i . α_i and h_i are species preferential diffusion coefficient for progress variable and enthalpy, respectively.

3. Results and discussion

3.1. Conditions and flame structure

In the current study, the target flame is methane flame, with an equivalence ratio of 0.8. The ammonia flame will be used to replace it in the same power condition (around 20kW), which is set up by three cracking ratio cases, i.e., Cr = 0.2, 0.4, and 0.6. The equivalence ratio is 0.9. The detail of the experiment and simulation conditions are described in Table 1.

Table. 1 Summary of experiment and simulation condition

ID	Composition	Cracking ratio %	Exp.	Sim.	U m/s	Power kW
1	CH ₄ /air ϕ = 0.8	-	✓	✓	10	20.8
2	NH ₃ /air ϕ = 0.9	0	✓		9.72	19.83
3	NH ₃ /H ₂ /N ₂ /air ϕ = 0.9	20	✓	✓	10.11	20.32
4	NH ₃ /H ₂ /N ₂ /air ϕ = 0.9	40	✓	✓	10.5	20.83
5	NH ₃ /H ₂ /N ₂ /air ϕ = 0.9	60	✓	✓	10.89	21.25

The instantaneous flame structure is depicted in Fig. 3, showing the digital photos (a) and the OH-PLIF figures (b). The methane flame shows a light blue color. The ammonia flame shows a yellow color caused by the NH₂α band [20]. There are OH signals both in the internal recirculation zone (IRZ) and outer recirculation zone (ORZ) for methane flame. As for pure ammonia flame, The OH signal is only distributed in the IRZ. When the cracking ratio increases, the flame will be more similar to methane flame until Cr = 0.4, which is the same as methane flame. Both flames show the M typical structure. In addition, the length of the flame decreases as more ammonia is cracked. This indicates that the propagation velocity is reinforced. When the cracking ratio reaches 0.6, the flame shows the flashback tendency. A more detailed comparison will be investigated in the following sections.

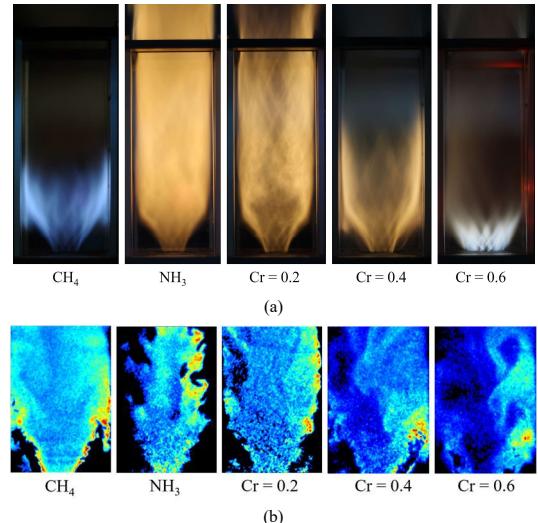


Figure 3 (a) Digital figure of the flame structure with 1/200s ISO 800. (b) OH-PLIF figure for methane and ammonia cracking cases.

3.2. Emission characteristic and wall temperature

Ammonia combustion is one of the carbon-free strategies. However, the NOx emission will sharply rise in ammonia flame because of the high nitrogen source in the fuel. NOx emission can be reduced during the reacting process or post-process. Several researchers pointed out that the NOx formation in fuel-rich conditions will be reduced in reacting process [4, 15]. While in the current study, to realize the complete combustion of fuel, we choose the equivalence equals 0.9.

The emission characteristics are shown in Fig. 4. With the increasing of cracking ratio, the unburnt ammonia is reduced. It is because there is more ammonia is cracked into hydrogen and nitrogen. And the combustion intensity is increasing meantime, resulting in the total consumption of ammonia. Other emissions, i.e., NO, N₂O and NO₂, show a monotonous increasing trend. As for the replacing condition, Cr = 0.4; although the power and flame structure characteristics are similar to methane flame, the deterioration of emission should be handled more carefully. An extra post emission process method, such as a Selective Catalytic Reduction system (SCR), should be set up.

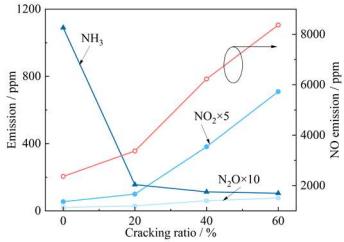


Figure 4 Emission performance of ammonia cracking flames measured by FTIR system

The wall mean temperature is also measured, which is shown in Fig. 5. The temperature in a stable condition of cases Cr = 0 ~ 0.6 is 513K, 743K, 978K, and 1010K, respectively. And the wall mean temperature of methane flame is 983K. The mean temperature of Cr = 0.4 case is close to methane flame. It is indicated that the heat release under the same flame structure is also similar between the methane case and replacing case (Cr = 0.4). This temperature data will also be used in the following LES study.

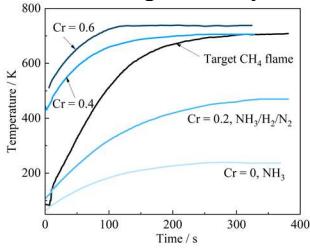


Figure 5 Wall temperature comparison

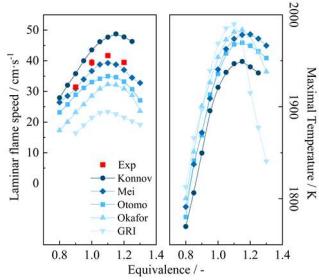


Figure 6 Comparison of the mechanism under the Cr=0.4 case's condition

3.3. Mechanism selection and 1-D simulation

To investigate why the Cr=0.4 alternative case is much similar to the methane case and give more fundamental support to such replacement. The 1-D and corresponding 3-D simulation will be carried out. First of all, a suitable reaction mechanism should be selected. For methane flame, the GRI 3.0 mechanism is used, verified in many studies. For the ammonia case, the calculation

condition is Cr = 0.4. Five mechanisms of ammonia are compared here through laminar flame speed and adiabatic temperature, shown in Fig. 6. The red points are experimental data for validation. It can be found that the Mei mechanism is the most agreement one, especially when equivalence is 0.9. The model also has been proved suitable for ammonia cracking conditions, i.e., NH₃/H₂/N₂/air flames [10]. Therefore, the Mei mechanism will be used following simulation research, which has 40 species [10].

Figure 7 shows the 1-D simulation map result of ammonia cracking cases. The x-axis is equivalence, and the y-axis is cracking ratio. The NOx emission is very high when the cracking ratio is around 0.7, especially under stoichiometric conditions. With an increasing of cracking ratio, thermal NO contributes more to the NO formation by the Zeldovich mechanism (N+O₂→NO+O, O+N₂→NO+N, N+OH→NO+H). The NH₃ emission is only prominent in low cracking ratio and fuel rich conditions. H₂ is more related to equivalence for cracking cases and mainly occurs in fuel rich conditions, which is from unburnt H₂ and converted from NH₃ through reactions between NH_x and H [21]. There is nearly no H₂ production in fuel lean conditions.

The flame speed, ambient temperature, and heat release rate are shown in the second line of Fig. 7. The red line is the corresponding value of the methane case. The red dots represent the ammonia cracking cases. From a comprehensive perspective, the Cr=0.4 case is similar to methane in these fundamental parameters. It indicates that the flame structure will be similar when we maintain the major basic parameters. Therefore, there will be an opportunity that the cracking ammonia flame can replace the methane flame with the same power.

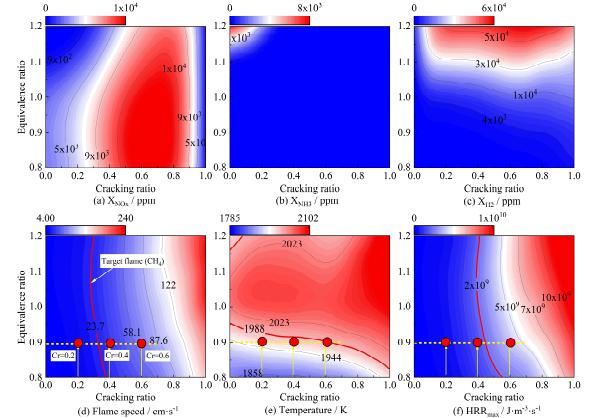


Figure 7 1-D premixed free NH₃ flame in different cracking ratio and equivalence ratio conditions. (a-c) emission, (d) Flame speed, (e) Temperature, (f) Heat release rate. The red line represents the target methane flame under $\phi = 0.8$. All the calculation is based on the 1 atmosphere and 300K.

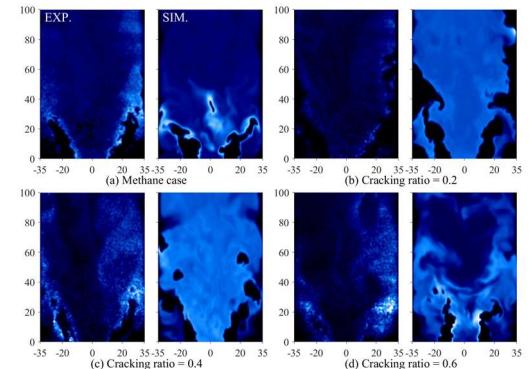


Figure 8 Comparison of OH-PLIF (right) and OH distribution calculated by LES (left)

3.4. Large eddy simulation and comparison of HRR

According to the 1-D simulation, ammonia cracking flame may replace methane case when the fundamental parameters are similar. This will give a more profound analysis of the replacement.

Therefore, the large eddy simulation coupled with the preferential diffusion FGM method will be carried out.

Figure 8 shows the good agreement of the OH field between the experiment and simulation. Figure 9 shows the scatter of temperature and heat release rate (HRR) and colored by the progress variable. The red line is the conditional average value of HRR. Compared with three ammonia cracking cases, the distribution of methane flame is very similar to ammonia flame under Cr=0.4. The maximum value of mean HRR is 1.05×10^9 J/s. And the corresponding temperature is around 1500 K. When the cracking ratio is smaller or larger than 0.4, the characteristic will be pretty different with methane flame, although they have the same power. As for the ammonia cases, it can be found that with an increasing of cracking ratio, the maximum value of HRR will also increase, indicating that cracking has a prominent influence on heat release rate. The corresponding temperature of maximum Hrr moves to low temperature conditions when cracking ratio increases. It is because the fresh mixture is more activated.

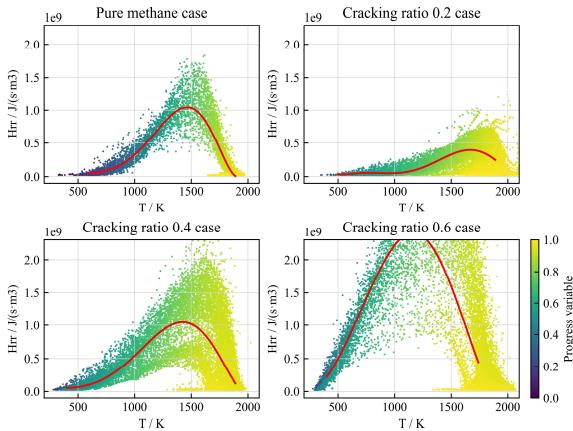


Figure 9 Instantaneous scatterplots of temperature versus heat release rate, colored by progress variable, which is defined in section 2.3

5. Conclusions

In this study, the possibility of using online cracking of ammonia to replace methane in a model gas turbine was investigated both experimentally and numerically. The experiment and large eddy simulation were carried out to compare the methane flame with the cracking ammonia flame. When the cracking ratio was around 0.4, the ammonia flame was more similar to methane one from flame structure, wall temperature, heat release, and other characteristics. The result gave the evidence for replacing methane by cracking ammonia and pointed out the suitable cracking ratio. However, the emission of ammonia flame was still really high. The post process system should be considered when using cracking ammonia to replace methane under the same power condition.

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