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# Influence of Doped H<sub>2</sub>O or H<sub>2</sub> on Soot Production and Power Capability in the Fuel-rich Gas Generator

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## ABSTRACT

Influence of doped H<sub>2</sub>O or H<sub>2</sub> on both soot production and power capability in the fuel-rich gas generator has been studied together by using the program of chemical equilibrium with applications (CEA). The oxidant is LOX, and the fuel is composed of Jet-A and the additive. The parameters of the gas generator are as follows: the range of combustion temperature is 800–1700 K, combustion pressure is 0.1–5.0 MPa, oxidant/fuel ratio is 0.1–1.2, and the mass percent of the additive in fuel is 0–60%. The results indicate that the addition of either H<sub>2</sub>O or H<sub>2</sub> can obviously reduce the mass percent of soot in combustion products, and the reasons are discussed on the base of the products distributions. Moreover, the minimum amounts of addition to surrender mass percent of soot less than 0.1% are present. The effects of combustion pressure on soot mass percent in combustion products appear turning appoints around 1100 K, no matter the additive is H<sub>2</sub>O or H<sub>2</sub>. The addition of H<sub>2</sub> can obviously improve the power capacity of combustion products in the whole temperature range. The addition of H<sub>2</sub>O can also improve slightly the power capacity of combustion products, when the combustion temperature is less than 1400 K. Effective molar weight of combustion products is the main factor affecting power capacity.

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Soot; fuel-rich combustion;  
gas generator; power  
capacity

## Introduction

In recent years, reusable rocket is a hot spot and a trend of space development at home and abroad, which can greatly reduce the cost of space launch (Donahue et al. 2008). The rocket engine system is the core of the rocket, and the gas generator cycle is one of the main cycle modes of the rocket engine. At present, the most popular reusable Falcon 9 rocket uses the Merlin series engine which employs the rich-fuel gas generator (Vozoff and Couluris 2008). For the LOX/kerosene rocket engine with gas generator cycle, the high concentration of soot and the large area of coke deposition in the pipeline (Edwards 2006) have adverse effects on the rocket engine system and structure, thus reducing the performance and operation life of the rocket engine. It is not conducive to the reuse of the rocket. Therefore, it is necessary to study influential factors on the formation mechanism as well as the amount of soot and coke deposition during the combustion of aviation kerosene. The relevant studies have been performed. In soot formation mechanism, Hai Wang (Wang

2011) reviewed the research status of sooting processes in the past 20 years, including soot precursor formation, particle nucleation, and mass/size growth. Formation mechanism of coke deposition, including the chemical processes of coke deposition formation and the factors affecting deposition content has been extensively studied (Beaver et al. 2005; Heneghan and Zabarnick 1994; Spadaccini, Sobel, Huang 2001). In the gas generator carbon deposition, the effects of mixture ratios and combustion pressure on soot formation and deposition characteristics were studied in a fuel-rich LOX/kerosene gas generator and a GOX/kerosene gas generator (Feng et al. 2017; Lausten, Rousar, Buccella 1985; Lawver 1983). The carbon deposition and soot formation characteristics of RP-3 kerosene under certain conditions were studied (Abdalla et al. 2020; Pei and Hou 2016), which indicates different types of kerosene also affect carbon deposition and the formation of soot. In addition, the development of numerical calculation also enables researchers to further study the characteristics of coke and soot (Foelsche et al. 1994; Yu and Lee 2007). For some hydrocarbon fuels, such as gasoline, the effects of the addition of alcohol and ether on the soot formation and combustion properties of the fuel were studied (Liu et al. 2018; Zhu et al. 2020), but as far as we know the additional components were rarely involved to suppress sooting in aviation kerosene and oxygen combustion. Moreover, influence of the additive on the power capability of combustion products of the gas generator were rarely studied.

Influence of doped  $H_2O$  or  $H_2$  on soot production and power capability of combustion products in the fuel-rich gas generator has been studied together in this work. Through calculation, effects of the additive amount of  $H_2O$  or  $H_2$ , oxidant/fuel ratio, and combustion pressure on soot mass percent in combustion products are analyzed, while their effects on the molar weight and the specific heat ratio of the combustion products, furthermore on the power capacity are also analyzed.

Calculation model

The soot can be oxidized by OH and O. Adding some other components such as  $H_2O$  and  $H_2$  to aviation kerosene during combustion in the fuel-rich gas generator may increase the content of OH and O in the combustion process so that the soot content in combustion products is reduced. Moreover, it will also affect power capacity of the combustion products. In order to study this, the thermodynamic calculation was carried out by utilizing the program of chemical equilibrium with applications (CEA) developed by NASA (Gordon and McBride 1994) in this paper.

Table 1 shows the parameters set in CEA calculation, and the corresponding calculation type is HP (Enthalpy and Pressure) type, in which the combustion pressure is constant. The composition of fuel and oxidant should be set in the calculation. Fuel is composed of Jet-A aviation kerosene and the additive, while the oxidant is liquid oxygen. In addition, the

Table 1. Parameters set in CEA calculation.

| Parameter                            |           | Parameter range        |                      |
|--------------------------------------|-----------|------------------------|----------------------|
| Combustion pressure, MPa             |           | 0.1, 1, 2, 3, 5        |                      |
| Oxidant                              |           | O2(L) $T_0=90$ K       |                      |
| Fuel                                 | kerosene  | Jet-A(L) $T_0=298$ K   |                      |
|                                      | additives | $H_2O$ (L) $T_0=300$ K | $H_2$ (L) $T_0=20$ K |
| Oxidant/Fuel ratio                   |           | 0.1–1.2                |                      |
| Mass percent of the additive in Fuel |           | 0%- 60%                |                      |

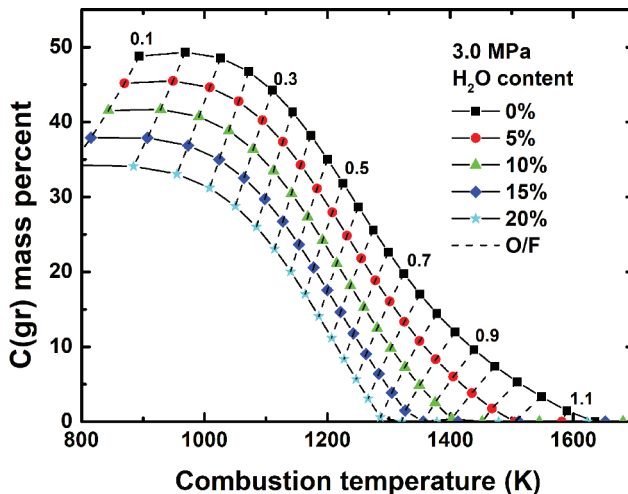
combustion pressure, oxidant/fuel ratio and initial temperature  $T_0$  of each component should be set. The thermodynamic data and calculation format are from User's Manual of CEA (Mcbride and Gordon 1996).

## Results and discussions

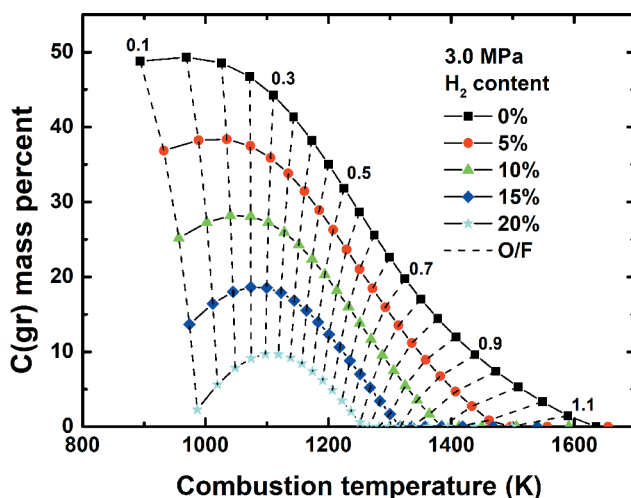
### *Influence of doped $H_2O$ or $H_2$ on soot mass percent in combustion products*

Figure 1 shows the trend of soot mass percent in combustion products with combustion temperature increasing in the range of 800–1700 K at different addition amounts of  $H_2O$ . The combustion pressure is 3.0 MPa. The oxidant/fuel ratios corresponding to the data points are also marked. In CEA, C(gr) is the condensed phase carbon in the combustion products, which is simply equivalent to soot in this work. It can be found that when the combustion temperature is less than 1000 K, the mass percent of soot changes little as combustion temperature changes. When the combustion temperature is over 1000 K, the mass percent of soot decreases remarkably with combustion temperature increasing. In addition, the variation trend with different addition amounts of  $H_2O$  is very similar. As the addition of  $H_2O$  in fuel increases, soot mass percent decreases obviously at the same combustion temperature. Compared with no  $H_2O$  addition, the addition of 20%  $H_2O$  can drop by about 15% soot mass percent at any fixed combustion temperature. For the same soot mass percent, the addition of 20%  $H_2O$  can drop the combustion temperature by about 200 K at least.

Figure 2 shows the trend of soot mass percent in combustion products with combustion temperature increasing in the range of 800–1700 K at different addition amounts of  $H_2$ . The combustion pressure is also 3.0 MPa. The oxidant/fuel ratios corresponding to the data points are also marked. It can be found that the more  $H_2$  added, the more obvious the trend of mass percent of soot increasing first and then decreasing as combustion temperature increases. The peaks are in the range of 1050–1100 K. As the  $H_2$  mass percent in fuel



**Figure 1.** Variation trend of soot mass percent with combustion temperature at different addition amounts of  $H_2O$ .

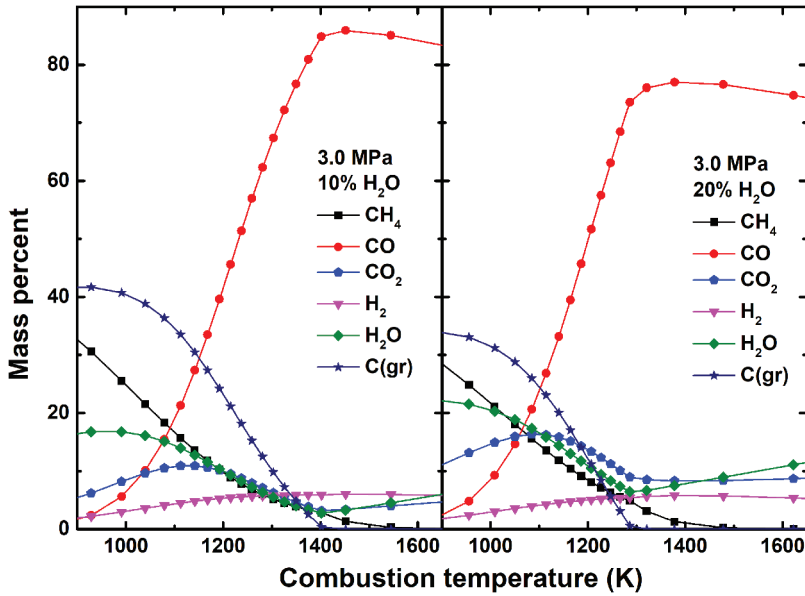


**Figure 2.** Variation trend of soot mass percent with combustion temperature at different addition amounts of H<sub>2</sub>.

increases, soot mass percent decreases obviously at the same combustion temperature. Compared with no H<sub>2</sub> addition, the addition of 20% H<sub>2</sub> can drop by over 30% soot mass percent at the same combustion temperature until there is no soot.

Compared with Figure 1, it can be seen that the trend of the soot mass percent with H<sub>2</sub> addition appears different. At low combustion temperature, such as less than 1200 K, adding H<sub>2</sub> can reduce the soot mass percent much more obviously than adding H<sub>2</sub>O at the same amount of addition. With the increase of combustion temperature over 1200 K, the reduction of soot mass percent decreases under the same increment of addition amount, and the trend of reduction of soot mass percent is similar to that when the additive is H<sub>2</sub>O. It implies that there are more than one dominant influential factor on soot mass percent, and the dominant factor may change with the temperature increasing. In addition, the influential factor may be same at the relative high combustion temperature.

In order to better understand the effects of additives on the soot mass percent, Figure 3 and Figure 4 respectively show the variation trend of the mass percent of six species in the combustion products with 10% and 20% two mass percents of the additive in fuel in the combustion temperature range of 800–1700 K. In Figure 3, the additive is H<sub>2</sub>O. When the combustion temperature is higher than 1100 K, the C(gr) and H<sub>2</sub>O mass percent in the combustion products decrease, while the mass percent of CO and H<sub>2</sub> increase, which indicates that there is an obvious water gas reaction to reduce soot. In Figure 4, the additive is H<sub>2</sub>. It can be found that there is a peak of soot mass percent around 1100 K, different from Figure 3. When the combustion temperature is less than 1100 K, the soot mass percent increases with the combustion temperature raising, and the H<sub>2</sub>O mass percent increases at the same time, which shows water gas reaction doesn't occur below 1100 K. CH<sub>4</sub> is one dominant product of Jet-A thermal decomposition, and it can further decompose to carbon and hydrogen with temperature increasing. The addition of H<sub>2</sub> can suppress the further decomposition of CH<sub>4</sub> thus reducing soot formation, which follows the le Chatelier's principle. With temperature increasing, the decomposition of CH<sub>4</sub> becomes more and more drastically, and the suppression effect on soot correspondingly

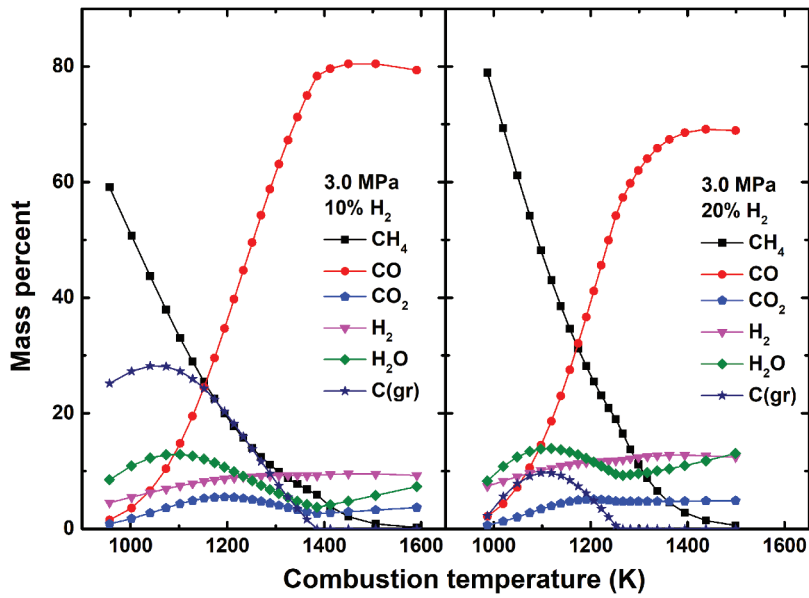


**Figure 3.** Variation trend of the mass percent of six species in the combustion products with combustion temperature (the additive is H<sub>2</sub>O).

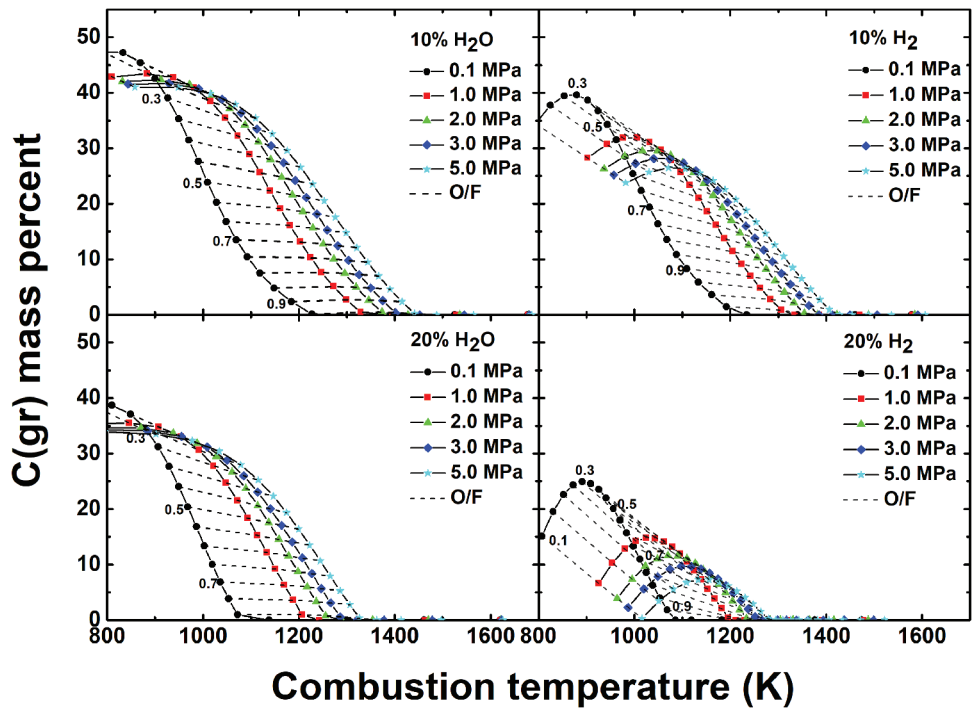
weaken its influence. Therefore, the soot mass percent increases with the temperature increasing. When the combustion temperature is more than 1100 K, there is an obvious water gas reaction, which is the same to that shown in Figure 3. With the development of water gas reaction and the increase of combustion temperature, soot begins to oxidize obviously, forming the peak of soot mass percent around 1100 K.

Figure 5 shows the effects of combustion pressure on soot mass percent in combustion products when the additives are H<sub>2</sub>O and H<sub>2</sub>, respectively. The range of combustion pressure is 1–5 MPa. Turning appoints appear around 1100 K for both H<sub>2</sub>O and H<sub>2</sub> addition. The influence of combustion pressure on soot mass percent is very small at different H<sub>2</sub>O mass percent in fuel at the combustion temperatures lower than 1100 K. When the additive is H<sub>2</sub>, the range of combustion pressure is 1–5 MPa and the combustion temperature is lower than 1100 K, the lower the combustion pressure, the higher the soot mass percent at the same combustion temperature. When the combustion temperature is more than 1100 K, the higher the combustion pressure, the higher the soot mass percent at the same combustion temperature, whether adding H<sub>2</sub>O or adding H<sub>2</sub>.

As shown above, it is worth doping either H<sub>2</sub>O or H<sub>2</sub> to suppress the sooting. Moreover, the required amount of addition to completely inhibit the soot is helpful to the designer of the gas generator. Figure 6 shows the mass percent of H<sub>2</sub>O required to drop the soot mass percent to 0.1%, while Figure 7 presents the required amount of H<sub>2</sub>. It is believed that the soot can be neglectable once its mass percent in combustion products is less than 0.1%. The required amount of H<sub>2</sub>O decreases with combustion temperature increasing and the trend is similar at different combustion pressures. At the same combustion temperature, the addition amounts of H<sub>2</sub>O required increases with the increase of combustion pressure. The mass percent of H<sub>2</sub>O drops from 60% to 0% as the combustion temperature from 800 K to 1700 K. The required



**Figure 4.** Variation trend of the mass percent of six species in the combustion products with combustion temperature (the additive is H<sub>2</sub>).



**Figure 5.** Effects of combustion pressure on soot mass percent in combustion products.

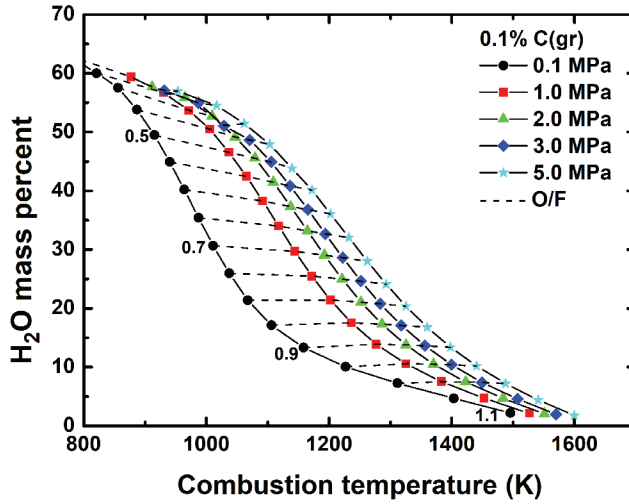


Figure 6. The mass percent of  $\text{H}_2\text{O}$  required to drop the soot mass percent to 0.1%.

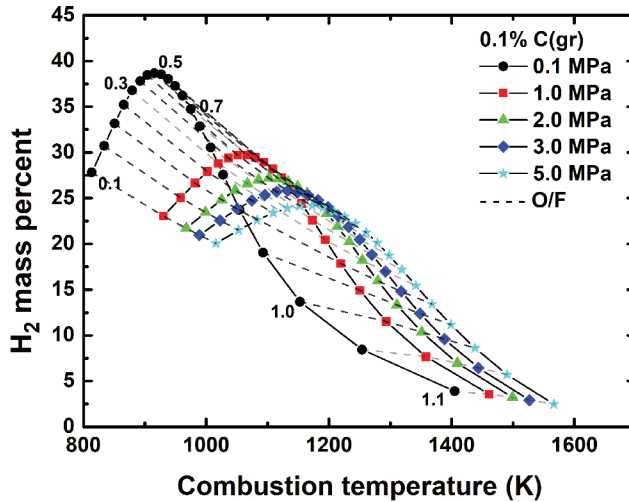


Figure 7. The mass percent of  $\text{H}_2$  required to drop the soot mass percent to 0.1%.

amount of  $\text{H}_2$  presents a different trend. In the typically employed combustion pressure range of 1–5 MPa, there is a boundary around 1180 K. Below this combustion temperature, the required mass percent of  $\text{H}_2$  is inversely proportional to the combustion pressure. It is exactly opposite above 1180 K. It can be explained by the same reason as mentioned above. Below 1180 K, high concentration of  $\text{H}_2$  in combustion process also inhibits the dehydrogenation reaction required for soot formation. According to le Chatelier's principle, when the combustion pressure increases, the suppression effect is enhanced. Above 1180 K, the increase of combustion pressure weakens the water gas reaction, thus it needs to increase reactant water, which results in the increase of addition amounts of  $\text{H}_2$ .



### ***Influence of doped H<sub>2</sub>O or H<sub>2</sub> on the power capacity***

Although the addition of either H<sub>2</sub>O or H<sub>2</sub> is helpful to restrain the sooting, it is not necessarily the more the better. Because influence of the addition on both the power capacity of combustion products and the fuel heat value should be considered. In this section, the effects of addition amounts of additives on the power capacity of combustion products will be analyzed. It is assumed that the combustion products flow isentropically, and the formula of its power capacity  $P$  is as follows:

$$P = \theta \dot{m} \Delta H = -\theta \dot{m} \int^V dp = \frac{\theta \dot{m} \gamma R T_1}{\gamma - 1} \left\{ 1 - \left( \frac{p_2}{p_1} \right)^{\gamma - 1/\gamma} \right\}$$

Where,  $\theta$  is the sum of the mass percent of the gas phase components in the combustion products,  $\dot{m}$  is the mass flow rate of combustion products,  $\Delta H$  is the change of enthalpy with the flow expanding isentropically,  $-\int^V dp$  is the expansion work of the gas phase components in combustion products,  $V$  is the gas volume per unit mass, and  $p$  is the pressure. There are both gas-phase components and condensed-phase components in the combustion products, and the condensed-phase components will not expand to do work. The gas-phase components of the combustion products are considered as an ideal gas whose specific heat ratio is  $\gamma$ . The gas constant of the ideal gas is  $R$ , which is equal to the universal gas constant  $R_0$  divided by the average molar weight  $M_g$  of gas-phase part in the combustion products. It is assumed that  $\gamma$  and  $R$  are invariant during the isentropic flow and  $\gamma$  is approximately equal to that of combustion products for the consideration of simplifying the analysis.  $T_1$  and  $p_1$  are the combustion temperature and the combustion pressure at the beginning of the isentropic flow, respectively, while the pressure at the end of the isentropic flow is  $p_2$ . The turbine efficiency is related to the specific turbine design and is not considered here.

It can be seen from above equation that power capacity is proportional to  $\theta$  and  $T_1$ , and inverse proportional to average molar weight  $M_g$  of gas-phase part, while the relation between the power capacity and the specific heat ratio  $\gamma$  is not straightforward.  $\theta$  is approximately equal to 1 minus the mass percent of soot in combustion products, on this basis, the formula of  $M_g$  is as follows:

$$M_g = \frac{\sum_{j=1}^{NG} n_j M_j}{\sum_{j=1}^{NG} n_j} = \frac{\theta}{\sum_{j=1}^{NG} n_j} = \theta M$$

$$M = \frac{\sum_{j=1}^{NS} n_j M_j}{\sum_{j=1}^{NG} n_j} = \frac{1}{\sum_{j=1}^{NG} n_j}$$

Where  $n_j$  is the number of kilogram-moles of species  $j$  per kilogram of combustion products, the index NG refers to the number of gases in the combustion products, NS refers to the total number of gases and condensed species, and  $M$  is defined as the effective average molar weight of the combustion products in isentropic expansion. In order to study the influence of specific heat ratio  $\gamma$  on the power capacity of combustion products, the function  $\alpha(\gamma)$  is constructed as follows:

$$\alpha(\gamma) = \frac{\gamma}{(\gamma - 1)} \left\{ 1 - \left( \frac{p_2}{p_1} \right)^{\gamma - 1/\gamma} \right\}$$

Then, the valuation formula of its power capacity  $P$  can be simplified as follows:

$$P = \frac{\dot{m} R_0 T_1 \alpha(\gamma)}{M}$$

The variation trends of power capacity  $P$  with combustion temperature  $T_1$  are given when  $p_1$  is a typical value 3.0 MPa,  $p_2$  is 0.3 MPa, and additives are  $H_2O$  and  $H_2$  respectively, as shown in Figure 8. Where, the trend of effective average molar weight  $M$  and the trend of  $\alpha(\gamma)$  are shown in Figure 9 and Figure 10, respectively. Specific heat ratio  $\gamma$  is assumed to be equal to specific heat ratio of combustion products, is 1000 g/s,  $R_0$  is 8.314 J/(mol · K).

It can be seen from Figure 8 that the power capacity of combustion products raises with the combustion temperature increasing. When the additive is  $H_2O$  and the combustion temperature is less than 1400 K, the power capacity of combustion products increases slightly as the addition of  $H_2O$  raises at the same combustion temperature. However, when the combustion temperature is more than 1400 K, the power capacity of combustion products at the same combustion temperature decreases slightly with the increase of the addition of  $H_2O$ . On the whole, the different amount of  $H_2O$  added has little influence on the power capacity of combustion products. When the additive is  $H_2$ , the power capacity of combustion products increases with the addition of  $H_2$  increasing at any point of the whole combustion temperature range. Compared with adding  $H_2O$ , adding  $H_2$  increases more the power capacity of combustion products under the same addition amount and combustion temperature.

Figure 9 and Figure 10 show the variation trend of effective average molar weight  $M$  of the combustion products with combustion temperature and the variation trend of  $\alpha(\gamma)$  with combustion temperature when the additives are  $H_2O$  and  $H_2$  respectively. The power capacities of combustion products are affected by the two factors  $M$  and  $\alpha(\gamma)$  at a given combustion temperature. In Figure 9, when the additive is  $H_2O$ ,  $M$  first decreases and then

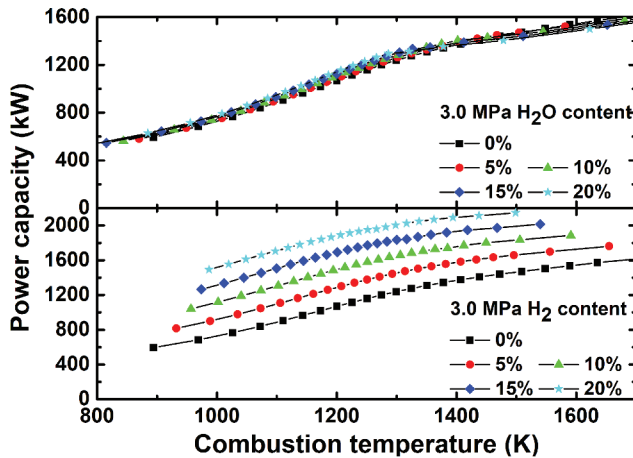
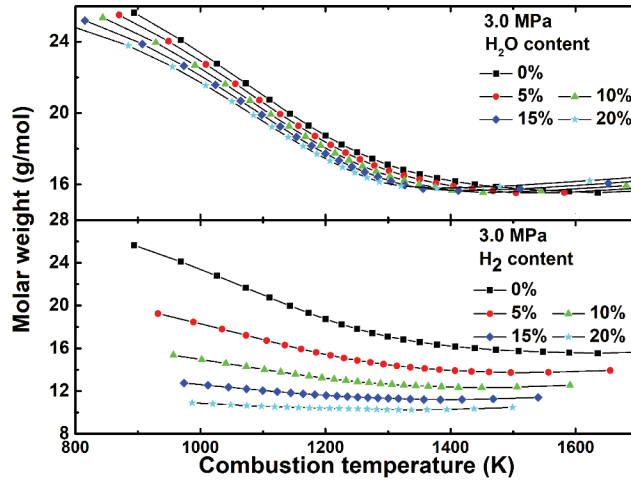


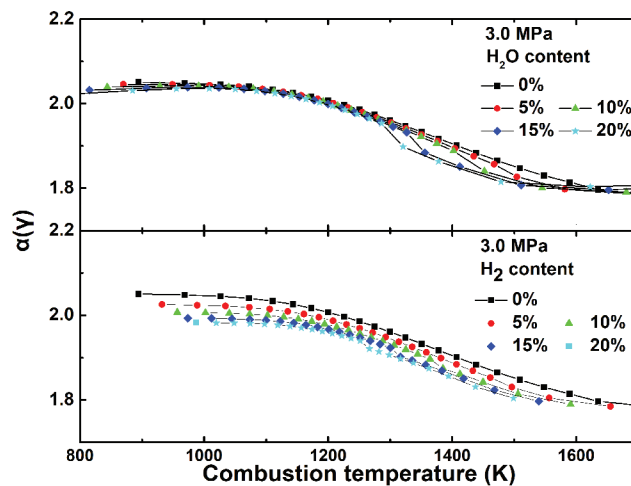
Figure 8. The variation trend of power capacity  $P$  with combustion temperature.



**Figure 9.** The variation trend of effective molar weight  $M$  of the combustion products with combustion temperature.

increases with the combustion temperature increasing. Moreover, more H<sub>2</sub>O added, the smaller  $M$  at the same combustion temperature less than 1400 K. When the additive is H<sub>2</sub>,  $M$  decreases first, then stabilizes with the increase of combustion temperature. Moreover, as added H<sub>2</sub> increases, the  $M$  obviously becomes smaller at the same combustion temperature in the study temperature range. Compared with adding H<sub>2</sub>O, adding H<sub>2</sub> can reduce the average molar weight  $M$  more, because H<sub>2</sub> has a smaller molar weight.

In Figure 10, whether the additive is H<sub>2</sub>O or H<sub>2</sub>,  $\alpha(\gamma)$  decreases with the increase of combustion temperature, and its value ranges from 1.8 to 2.2. At the same combustion temperature and inlet and outlet pressure, the parameters affecting power capacity  $P$  are  $\Delta M/M$  and  $\Delta\alpha(\gamma)/\alpha(\gamma)$ . It can be seen from Figure 9 and Figure 10 that the value of



**Figure 10.** The variation trend of  $\alpha(\gamma)$  with combustion temperature.

$\left| \frac{\Delta\alpha(\gamma)/\alpha(\gamma)}{\Delta M/M} \right|$  is remarkably less than 1, so the  $M$  is the main factors affecting  $P$ . The influence of  $M$  on the power capacity is slightly weakened by the specific heat ratio  $\gamma$ .

## Concluding remarks

In this paper, influence of doped  $\text{H}_2\text{O}$  or  $\text{H}_2$  on both soot production and power capability in the fuel-rich gas generator has been studied together in the temperature range of 800–1700 K, combustion pressure range of 0.1–5.0 MPa. It is found that both  $\text{H}_2\text{O}$  and  $\text{H}_2$  as the additive in fuel can reduce soot mass percent, and  $\text{H}_2$  addition can obviously improve the power capacity of combustion products. The water gas reaction plays the key role on the soot reducing above 1100 K. Moreover, the effects of  $\text{H}_2\text{O}$  and  $\text{H}_2$  on the soot mass percent in the combustion products are different below 1100 K, and addition of  $\text{H}_2$  reduces the soot mass percent by preventing the further decomposition of  $\text{CH}_4$ , while addition of  $\text{H}_2\text{O}$  has no influence on the soot mass percent. The effects of combustion pressure on soot mass percent appear turning appoints around 1100 K for both  $\text{H}_2\text{O}$  and  $\text{H}_2$  addition. The soot mass percent in combustion products increases with the combustion pressure increasing at the same combustion temperature over 1100 K, no matter the additive is  $\text{H}_2\text{O}$  or  $\text{H}_2$ . The effect of the pressure appears opposite for  $\text{H}_2$  addition at the temperature less than about 1100 K, while the effect of the pressure is weak for  $\text{H}_2\text{O}$  addition. The effects of  $\text{H}_2\text{O}$  and  $\text{H}_2$  on the power capacity of combustion products are also not the same. The influence of  $\text{H}_2\text{O}$  addition on the power capacity of combustion products is slight, while  $\text{H}_2$  addition can obviously improve the power capacity. The differences are due to the different effects of additives on the effective molar weight and specific heat ratio of the combustion products. Effective molar weight of combustion products is the dominant factor affecting power capacity.

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