Entropy generation analysis of premixed hydrogen-air combustion in a micro combustor with different mass-flow velocity

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Abstract. In order to improve the flame stability in the micro combustor with a backward-facing step, porous media is being used in the combustion chamber. In this work, lots of analysis of entropy generation rate caused by chemical reaction, heat conduction and mass diffusion had been carried out. The effects of mass-flow velocity are numerically investigated via the analysis of entropy generation rate. Analysis in this paper reveal that: as the mass-flow velocity \( m_{H2}=1.13\times10^{-6}\text{kg/s} \), the micro combustor with porous media obtained the highest mean wall temperature and entropy generation rate \( 2.11\times10^{-3}\text{W/K} \). It is obviously seen that a higher mass-flow velocity contributes to a higher entropy generation rate and combustion efficiency.

1. Introduction

Nowadays, the urgent demand of the high power density, reliable, light-weight and efficient energy device has made Micro Electro Mechanical Systems (MEMS) become a research focus[1]. Micro thermo photovoltaic systems (MTPV) also attract much attention as a representative micro-mechanical device[2]. A high and uniform flame temperature is desirable for achieving a higher efficiency for the system[3]. Micro combustor is a core part of the MTPV system. It has been found that setting porous media inside the combustor can increase the average temperature and stability of the combustion[4]. J. Pan[5] investigated the effect of materials and porosity of porous medium to micro combustors. As an intuitive method to evaluate the performance on consuming energy, entropy generation has been used[6]. Dongyue jiang[7] made the first systematic analysis of the volume entropy generation rate. It has been found that the entropy yield induced by the chemical reaction increased with the increase of the flow rate, but as the CO mass fraction decreased, the increased flow rate had an effect of increasing the heat conduction which will lead to an increase in entropy yield. H. Herwig[8] found that chemical reaction dominates the total entropy generation rate, followed by thermal conduction.

The objective of this study is to investigate the influence of different mixture mass-flow velocity for combustors. Entropy generation rate has been calculated to show the energy consumption in the combustor intuitively. Temperature and mole fraction of OH radical distribution are also obtained for the research of the combustion performance.

2. Numerical models and Simulation approach

2.1. Physical and numerical model

A 3-D micro-cylindrical combustor using FLUENT has been employed for the research of entropy
generation. The schematic diagram of the micro combustor is shown in Fig.1. It is a cylindrical tube with an outer diameter of 7 mm, and the tube length is 27 mm. The combustor chamber is divided into the inlet section and the chamber after the backward-facing step, where the porous media is fully compacted. The inlet section length is 7 mm with a diameter of 2 mm. The diameter of the combustion chamber is 6 mm, and combustor wall thickness is 0.5 mm. Besides, the combustor is made of stainless steel 316 L with an emissivity of 0.78. Porosity of porous media is 0.72. The fluid regime is assumed to be Turbulent because of the backward-facing step and the porous media. The standard k-ε model, EDC model and the steady model are employed with a detailed hydrogen-air combustion chemical reaction mechanism which includes 9 species and 19 reactions. P1 radiation is also used for the radiation from internal porous media.

![Fig 1. Schematic of the micro combustor with porous media.](image)

2.2. Grid independency study
Three different mesh designs are investigated to obtain a grid-independent solution. 500000, 1100000 and 2000000 cells are employed shown in the Fig 2(a). It is obviously that the wall temperature is almost constant when the number of cells greater than or equal to 1100000. Hence, 1100000 cells for the mesh are employed to get a better precision.

2.3. Entropy generation
The volumetric entropy generation rate due to chemical reaction, thermal conduction and mass diffusion can be described as follows:

\[
S_{\text{gen, chemical}} = -\frac{1}{T} \mu_m r_m \tag{1}
\]

\[
S_{\text{gen, conductive}} = -\frac{1}{T^2} k (\nabla T)^2 \tag{2}
\]

\[
S_{\text{gen, diffusion}} = \sum_{m=1}^{n} (\rho R_{\text{g,m}}) \nabla Y_m \cdot \nabla X_m \tag{3}
\]

Total entropy generation rate:

\[
S_{\text{gen, total}} = \int_V (S_{\text{gen, chemical}} + S_{\text{gen, conductive}} + S_{\text{gen, diffusion}}) \, dv \tag{4}
\]

3. Results and analysis

3.1. Model validation
To validate the numerical model, experiments were carried out. Fig 2.(b) shows the comparison of experimental data and numerical simulation on the wall temperature of micro combustor at \( m_{H_2} = 7.50 \times 10^{-7} \text{kg/s} \). The equivalence ratio \( \Phi \) is kept as 0.9. It is obvious that a good agreement has been achieved which indicates the numerical simulation is right. As can be observed from Fig 2.(b), the temperature rises rapidly near the inlet and the highest wall temperature is obtained at 7 mm of combustor where the combustion reaction takes place. Then it decreases gradually due to the energy loss of heat convection and radiation.
3.2. Effects of mass flow velocity
A classic micro combustor made of steel 316 L and inserted with porous medium has been employed in this paper. Thermal performance and entropy generation are investigated to discuss effects of hydrogen-air mass-flow velocity to combustion. Three different hydrogen mass flow rates $7.50 \times 10^{-7}$ kg/s, $9.38 \times 10^{-7}$ kg/s, and $1.13 \times 10^{-6}$ kg/s are involved and the equivalence ratio is kept as 0.9. Fig. 3 shows Temperature and mole fraction of OH radical distribution at YZ plane of the combustor with porous media for different mass-flow velocity. The temperature distribution is more uniform and the OH radical increases when the mixture of hydrogen and air increases. The main reason for the phenomenon is that the increase in mass-flow velocity causes more oxygen and hydrogen to consume so that the hydrogen is fully burned. It also can be seen that the high temperature region and OH radical concentration move towards the outlet quickly.

Fig. 4 demonstrates that the effects of mass-flow velocity on the combustor with inserted porous media on the centerline volumetric entropy generation and the total entropy generation rate are induced by heat diffusion, mass diffusion and chemical reaction. It shows that profiles of the centerline volumetric entropy generation are increased and then decreased along the flow direction. Moreover, the
volumetric entropy generation rate mainly occurs at the inlet parts or middle section of the combustors, where the peak value of these profiles are located at $z < 10$ mm, and the other parts of the profile is 0. It is demonstrated that the location of high volumetric entropy generation zone moves to the outlet in Fig 4.(a) while it shifts to the inlet in Fig 4.(b) and (c). Different from the Fig 4.(a), the peak entropy generation rate value caused by heat conduction and mass diffusion gradually decreases with the increasing of the mass flow rate in Fig 4.(b) and (c). The high mass-flow velocity increases the flame temperature in the combustor and it also contributes to a higher entropy generation rate. Combining the “Eq.(4)” and the Figs, it can be revealed that the entropy generation rate caused by chemical reaction dominates the total entropy generation rate. According to “Eq.(2)” and “Eq.(3)”, the volumetric entropy generation caused by thermal conduction and mass diffusion is proportional to the gas temperature gradient and reaction species’ fraction gradient, respectively. It means that the mass-flow velocity of combustor affects the thermal performance, which changes the combustion reactions according to Arrhenius equation. As can be seen from the Fig 4.(d), the total entropy generation rate is $2.11 \times 10^{-3}$ W/K when the mass-flow velocity is $1.13 \times 10^{-6}$ kg/s.

![Fig 4. Volumetric entropy generation rate caused by (a) chemical reaction, (b) heat conduction and (c) mass diffusion and (d) total entropy generation rate in the combustor with porous media at $m_{H2}=7.50 \times 10^{-7}$ kg/s, $9.38 \times 10^{-7}$ kg/s, and $1.13 \times 10^{-6}$ kg/s and $\phi=0.9$.](image)

### 4. Conclusions

A 3-D micro-cylindrical combustor with porous media is established and verified by experiments. The following conclusions are summarized.

1. The increasing mass-flow velocity influences the wall temperature distribution. Locations of the high flame temperature zone and OH radical concentration move to the outlet when the mass-flow velocity increases. Mean wall temperature of the combustor would also increase.

2. The variation of entropy generation rate for the combustor is in agreement with the mean wall temperature as the mass-flow velocity increases. The entropy generation rate induced by chemical reaction increases as the mass-flow velocity increases, resulting in the increase in total entropy generation rate. When the mass-flow velocity is $1.13 \times 10^{-6}$ kg/s, the combustor gains the highest total
entropy generation rate $2.11 \times 10^{-3}$W/K.

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