A Numerical Investigation on Non-premixed Catalytic Combustion of CH_4/Air in a Symmetrical Planar Micro-combustor

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1 Introduction

As the energy density of typical hydrocarbon fuels is dozens of times that of traditional chemical batteries, there is a great potential for the development of combustion based micro power systems, such as micro engines, micro thrusters, micro TPV and so on. However, great challenges to flame stability also exist due to the large surface-to-volume ratio of micro-combustors. Many strategies have been put forward to promote flame stability. Catalytic combustion is one of the feasible methods, which has been proved effective in premixed micro combustion by numerous researches. Deutschman et al. [1] carried out numerical simulations for the catalytic ignition of CH_4, H_2 and CO on Pt and Pd surfaces, which showed a quantitative agreement between measured and calculated ignition temperatures. Pizza et al. [2] numerically demonstrated that flame instabilities in 1-mm and 2-mm height channels can be inhibited by varying the catalytically-active area. Yang et al. [3] showed that application of catalyst increased the power output of micro-TPV systems by 11%-23.8%. Chen et al. [4] revealed that transport properties played a significant role in determining catalytic combustion stability.

However, to the authors' knowledge, non-premixed catalytic combustion in micro channels has not been reported so far. In our previous work [5], we have validated the feasibility of non-premixed catalytic combustion in asymmetric micro-channels. The results showed that catalytic reactions mainly occurred in the fuel side and the combustion efficiency is relatively low (<77%). Therefore, in the present work, we designed a symmetrical micro-channel aiming at improving the combustion performance. The effects of inlet velocity and nominal equivalence ratio on the characteristics of non-premixed CH_4/air catalytic combustion were numerically investigated.

2 Numerical method

2.1 Geometric model

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A two-dimensional geometric model was adopted in this work. The geometric structure of the planar micro-combustor is schematically depicted in figure 1. The total length (L_0), channel height (H_0) and wall thickness (W_0) are 16 mm, 1.2 mm and 0.2 mm, respectively. The channel entrance is symmetrically divided into three parts by two separating plates with a length of L_1= 2 mm and a thickness of W_1= 0.2 mm. The upper and lower parts (H_2= 0.2 mm) are inlet ports for CH_4, while air is injected into the channel from the middle part (H_1= 0.4 mm). The inner wall surface of the micro-combustor is coated with Pt.

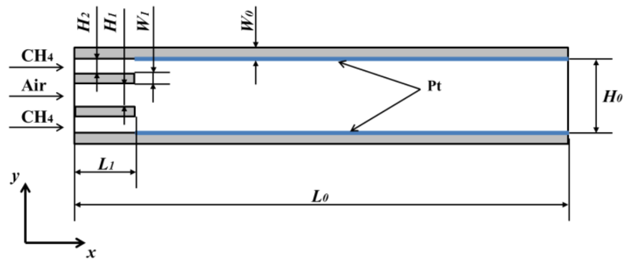


Figure 1. Schematic diagram of the catalytic planar micro-combustor

2.2 Computation scheme

The flow under investigation lies in the laminar regime. The governing equations were solved with popular CFD software, Fluent 14.0. The C1 reaction mechanism [6], consisting of 18 species and 58 elementary reactions, was employed for gas-phase combustion of CH_4/air. Meanwhile, the heterogeneous reaction mechanism proposed by Deutschmann et al. [1] with 11 surface species, 7 gas species and 24 elementary reactions was applied to simulate the catalytic reaction on Pt surface. The thermodynamic and kinetic parameters of all species were obtained from the CHEMIKIN database. Natural convection heat transfer and thermal radiation through channel outer wall surfaces to the surroundings were taken into account. The natural convection heat transfer coefficient is 20 W/(m^2·K) in this work, evaluated by outer wall temperature and Ref. [7], and the emissivity of the material (steel) is 0.2. Grid independence was verified by comparing predicted results using different grid systems and the grid size with Δx=Δy= 25 μm was employed in the final computation. As there is no experimental report on non-premixed micro catalytic combustion in the literature, comparison between the numerical results and experimental data cannot be made at present. Fortunately, the reaction mechanisms used in this work have been verified in premixed micro combustion [1, 8, 9] and widely employed in numerical investigation [10, 11]. Therefore, the results obtained in the present study are reliable.

3 Results and discussion

In this study, ϕ denotes nominal equivalence ratio (a global equivalence ratio, assuming fuel and oxidant are fully mixed), and $V_{ave,cold}$ means the average velocity of cold mixture in the channel, which is used to represent the inlet velocity. Combustion efficiency is defined as the ratio of the actual total heat release to the possible maximum heat release. Considering the main combustible components in the exhaust gas are CH_4, CO and H_2, η is calculated through Eq. (1):

$$\eta = 1 - \frac{m_{out,CH_4}\Delta h_{CH_4} + m_{out,CO}\Delta h_{CO} + m_{out,H_2}\Delta h_{H_2}}{m_{in,CH_4}\Delta h_{CH_4}} \quad (1)$$

where m_{in,CH_4} is the mass flow rate of CH_4 at the entrance, m_{out,CH_4}, $m_{out,CO}$ and m_{out,H_2} denote the mass flow rate of CH_4, CO and H_2 at the combustor exit, while Δh_{CH_4}, Δh_{CO} and Δh_{H_2} are the reaction enthalpies of CH_4, CO and H_2, respectively.

In genral, as catalytic reactions occur on the inner surface of the channel walls, the combustor has a high temperature level with a uniform temperature distribution, which is beneficial to micro-TPV devices. Thus, the applicability of the combutor for micro-TPV is assessed. Radiation efficiency, which is used to examine the energy conversation efficiency for micro-TPV, is defined as the ratio of the radiant energy output from exterior wall surfaces to the total chemical energy input.

Firstly, non-premixed CH_4/air catalytic combustion were simulated by using different reaction mechanism schemes (i.e., both homogeneous and heterogeneous, homogeneous alone and heterogeneous alone) to validate the contribution of homogeneous and heterogeneous reactions to CH_4 combustion. It comes out that pure homogeneous reactions can't occur in this channel because the channel height is much less than the quenching distance (about 2.5 mm) of CH_4/air combustion. The differences in results obtained by using both-homogeneous-and-heterogeneous and heterogeneous-alone reaction mechanisms are all within 1%, indicating that heterogeneous reactions play a major role in CH_4 combustion in the present configuration. However, for a higher prediction accuracy, both homogeneous and heterogeneous reaction mechanisms are adopted in our simulation.

3.1 Effects of inlet velocity on non-premixed CH_4/air catalytic combustion

In this section, ϕ is fixed at 1 and the effects of inlet velocity on non-premixed CH_4/air catalytic combustion are examined numerically. Temperature fields of the micro-combustor at different inlet velocities are illustrated in figure 2(a). It can be seen that with the increase of inlet velocity, temperature in the micro channel rises and the high temperature region on the channel wall expands. This is because as $V_{ave,cold}$ rises, the mass flow rates of fuel and air increase and total heat release by chemical reactions increases. Meanwhile, the position of maximum wall temperature moves downstream owing to the prolonged moving distance of O_2 at a large inlet velocity in an almost invariable diffusion time. These physics can also be explained by figure 2(b), which shows heat release rate (HRR) per unit length on the catalytic walls at different inlet velocities. It is noted that there is little difference on the peak values of heat release rate, whereas the position of the peak moves downstream with an increasing inlet velocity. It is also observed that although the heat release rate for lower inlet velocity is larger in the upstream region, it is reversed in the downstream region and the total heat release is much larger at a high inlet velocity.

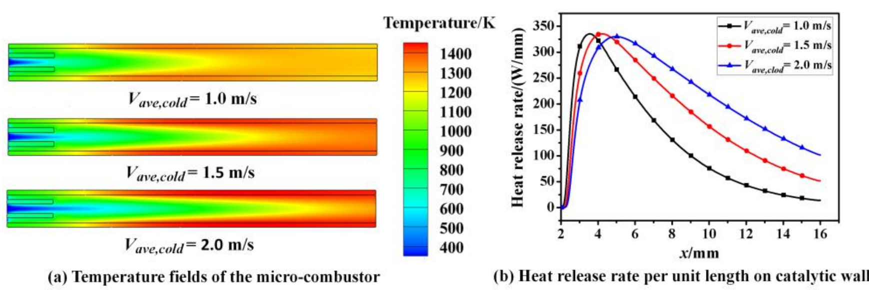
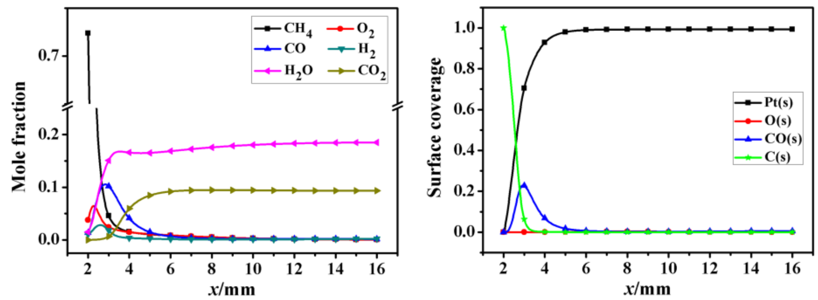


Figure 2. Temperature field and heat release rate per unit length on the catalytic wall at different inlet velocities

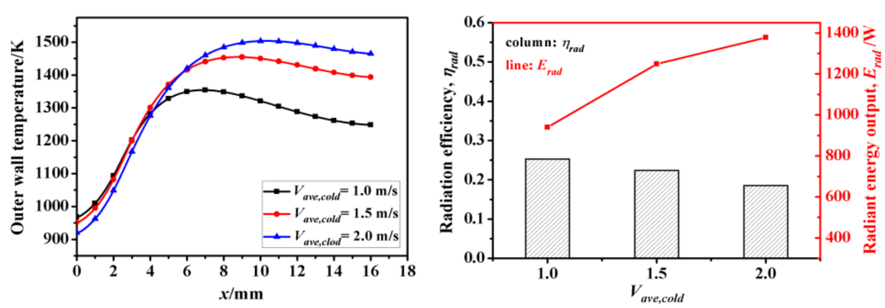
The concentration of major species near inner wall and the surface coverage of main species on catalytic wall are plotted in figure 3 for $V_{ave,cold}$= 1.0 m/s. It is shown in figure 3(a) that CH_4 are consumed quickly at the leading edge of catalytic wall. The concentration of O_2 increases first and then decreases, which is determined by the relative magnitude of diffusion velocity and reaction rate. In the upstream channel, the amount of O_2 is relatively insufficient, thus, CO is the main production of catalytic reactions with a small amount of H_2. It is noted that the position where CO_2 concentration increases steeply is 1 mm behind that of H_2O, and is consistent with that of CO concentration reduction. Figure 3(b) shows that the major surface species are C(s), Pt(s) and CO(s) at the leading edge of catalytic wall, while the surface coverage of Pt(s) is close to unity on the midstream and downstream channel wall, which is beneficial to the adsorption and reaction of CH_4. At the leading edge of catalytic wall, C(s) is formed by CH_4 dehydrogenation. With the diffusion of O_2, C(s) is oxidized to CO(s) and finally CO_2 is produced. This process is reflected more clearly in a non-premixed catalytic combustor than in a premixed catalytic combustor. The surface coverage of O(s) is extremely low in the whole channel inner wall, which differs from the typical characteristic of premixed catalytic combustion [10]. The coverage of O(s) on catalytic wall can inhibit the adsorption of CH_4, which further suppresses catalytic reactions. Therefore, a low surface coverage of O(s) is favorable to catalytic combustion. In addition, slight fuel rich condition is good for catalytic combustion [10]. This means the symmetrical configuration of this catalytic combustor, which can create a fuel rich condition near the catalytic wall surfaces, favors the catalytic combustion.



(a) Mole fraction of main species near catalytic wall (b) Surface coverage of main species on catalytic wall

Figure 3. Distributions of main species near the catalytic wall and on the catalytic wall surface

The lower velocity limit of this micro-combustor at ϕ= 1 is 0.7 m/s ($V_{in,air}$= 1.9004 m/s, $V_{in,CH4}$= 0.1996 m/s). The combustion efficiency decreases with the increase of inlet velocity and the maximum combustion efficiency is 97.6%. The combustion efficiency decreases to 80.4% at $V_{ave,cold}$= 2.0 m/s. Figure 4(a) shows the temperature distributions of the exterior wall surface at different inlet velocities. It can be seen that the downstream wall temperature increases as $V_{ave,cold}$ rises and the temperature change is relative gentle. The maximum outer wall temperature is about 1500 K at $V_{ave,cold}$= 2.0 m/s. Therefore, the high temperature and uniform distribution of this micro-combustor are fit for micro-TPV devices. The radiation efficiency and radiant energy output from external wall at different inlet velocities are depicted in figure 4(b). It is shown that with the increase of $V_{ave,cold}$, the radiant energy output increases while the radiation efficiency decreases. The radiation efficiencies at $V_{ave,cold}$= 1.0 m/s, 1.5 m/s and 2.0 m/s are 25.3%, 22.4% and 18.5% , respectively. As $V_{ave,cold}$ increases from 1.0 m/s to 1.5 m/s, the radiant energy output is increased by 32.9% while there is only a little decrease in radiation efficiency. Therefore, $V_{ave,cold}$= 1.5 m/s may be the best operation condition among the three cases for micro-TPV devices based on a comprehensive consideration.



(a) Temperature distribution on channel outer wall surface (b) Radiation efficiency and radiant energy output

Figure 4. (a) Temperature distribution on exterior wall surface; (b) radiation efficiency and radiant energy output from external wall surfaces at different inlet velocities

3.2 Effects of nominal equivalence ratio on non-premixed CH_4/air catalytic combustion

In this section, keeping $V_{ave,cold}$ at 1.5 m/s, the effects of nominal equivalence ratio on non-premixed CH_4/air catalytic combustion are examined by a comparison between ϕ= 0.9, 1.0 and 1.2. Because combustion can't be maintained at ϕ= 0.8, ϕ= 0.9 is chosen to represent the fuel lean condition.

The profiles of heat release rate per unit length on the catalytic wall at different nominal equivalence ratios are plotted in figure 5. It is demonstrated that although HRR at ϕ= 0.9 is a little higher in the upstream channel (x< 5 mm), there is a sharp decline at about x= 5.1 mm. Moreover, the HRR for ϕ= 1.0 is the highest on the midstream and downstream catalytic wall, followed by the case of ϕ= 1.2 and ϕ= 0.9. The steep decrease of HRR at ϕ= 0.9 results in a decline of O_2 consumption, thus, there is an increase in the O_2 mole fraction profile at x= 5.1 mm for ϕ= 0.9, as shown in figure 6(a). For a clearer observation, the mole fraction contour of O_2 for ϕ= 0.9 is illustrated in figure 6(b). In the upstream channel, there is an accumulation of O_2 near the inner walls due to species diffusion. As catalytic reactions occur, O_2 concentration decreases steeply and a relatively large outward concentration gradient forms. With the decline of reaction intensity, the outward diffusion of O_2 leads to a rebound in the O_2 concentration near the inner walls. The increase of O_2 concentration near the catalytic wall leads to a drastic rise in the surface coverage of O(s), as demonstrated in figure 7. As can be seen, for the cases of ϕ= 1.0 and 1.2, the catalytic wall surfaces are mainly coated by Pt(s) and the coverage of O(s) is close to zero on the whole catalytic wall, which is beneficial to catalytic reactions. However, for ϕ= 0.9, the surface coverage of O(s) is above 0.3, which in turn inhibits the absorption of CH_4 and reduces the catalytic reaction intensity. The decrease of HRR also decreases the wall temperature level, which further increases the surface coverage of O(s). The interactions of these factors results in the different combustion characteristics in fuel lean condition.

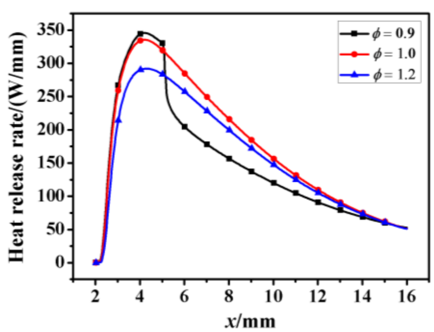


Figure 5. Heat release rate on catalytic wall at different nominal equivalence ratios

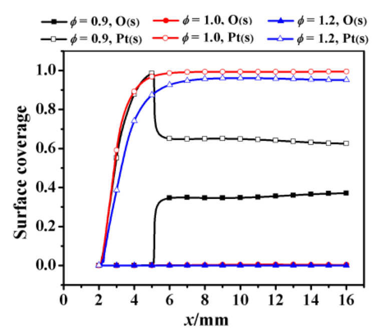


Figure 7. Surface coverage of Pt(s) and O(s) on catalytic wall

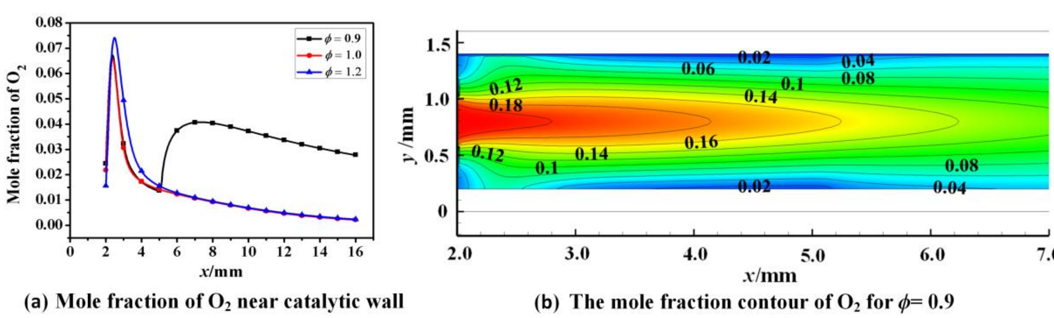


Figure 6. (a) O_2 mole fraction profiles near catalytic wall; (b) the O_2 mole fraction contour for ϕ= 0.9

Finally, the combustion efficiency and radiation efficiency for different nominal equivalence ratio are compared. It comes out that the combustion efficiency for ϕ= 1.0 is the highest (89.4%), followed by that of ϕ= 0.9 and ϕ= 1.2, which differs from the trend found in the asymmetric configuration [5]. The radiant energy output and radiation efficiency for ϕ= 0.9, 1.0 and 1.2 are 932.2 W, 1248.0 W, 1014.2 W and 18.4%, 22.4%, 15.4%, respectively. Therefore, ϕ= 1.0 may be the best choice for micro-TPV devices among the three scenarios.

4 Conclusions

The non-premixed catalytic combustion characteristics of CH_4/air in a symmetrical planar channel are numerically studied in the present work. It is found that with the increase of inlet velocity, the maximum temperature, total heat release rate and radiant energy output increase, whereas the combustion efficiency and radiation efficiency decrease. Moreover, a sharp increase in the surface coverage of O(s) on the catalytic wall and a decrease in the heat release of chemical reactions are observed in fuel lean case, which means that fuel lean condition may be not suitable for non-premixed catalytic combustion. Furthermore, this combustor shows satisfactory performance in combustion efficiency and radiation efficiency in a wide operation range, which benefits from the fuel rich atmosphere near the catalytic wall surfaces.

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