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# Numerical investigations on characteristics of methane catalytic combustion in micro-channels with a concave or convex wall cavity



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#### ABSTRACT

Catalytic combustion characteristics of methane in micro-channels with a concave and convex cavity, respectively, and in straight channel without cavity were numerically investigated. The results show that as the equivalence ratio ( $\phi$ ) increases, the methane conversion increases first and then decreases, the highest methane conversion ratio, which is 85.3%, occurs at  $\phi = 1.0$  in the micro-channel with convex wall cavity. The micro-channel with concave wall cavity is not conductive to methane catalytic micro-combustion at relatively low velocity. With the inlet velocity increasing, the methane conversion ratio is decreased. In the micro-channel with convex wall cavity, the inner wall pressure increases, because the fuel is disrupted when it flows through the cavity. Then the mixture of methane contact with catalyst is enhanced, which favors the combustion of methane. The recirculation zone which is the largest area formed in the micro-channel with convex wall cavity absorbs more high temperature gas and raises the combustion temperature. Heat transfer in the convex micro-channel is enhanced which makes the temperature distribution more uniform. The maximum value of the extinction limit is 16.5 m/s, which occurs in the micro-channel with convex cavity.

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#### 1. Introduction

Various small devices and systems are continuously emerging for military, industrial applications. As a core equipment of power micro-electromechanical systems (Power MEMS), many researchers have done a lot of researches on it [1-4]. About the definition of micro-scale, Ju and Maruta [5] discussed in recent research. They summarized that in order to avoid confusion with meso-scale, micro-scale was defined by choosing three length scale which were the physical dimension of the combustive reactor, the quenching diameter of flame and the relative length scale of the entire device to that of conventional large scale devices. First, if the combustor physical length scale was less than 1 mm, it was called microcombustion. If the physical length scale was more than 1 mm, it was called meso-combustion. Physical definition was widely adopted in micro-engines [6]. Second, if the radial size of combustor was less than the quenching diameter, it was called micro-scale combustion. If not, it was called meso-combustion. The quenching diameter of flame naked more sense in terms of physical flame

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regimes and was adopted by researchers for fundamental studies of micro-combustion. The third one was adopted to create microthrusters for specific applications [7]. According to the second definition, the quenching diameter of flame is usually very short, for example, the H<sub>2</sub> is 0.64 mm and CH<sub>4</sub> is 2.5 mm [8]. In the studies of micro-combustion, the size of micro-scale combustor, which is limited to the quenching diameter, decreases obviously. Because of the reduction of reaction chamber size, a series of problems appears. The large surface area-to-volume gives rise to higher heat loss. Combustion efficiency decreases due to the shortage of fuel residence time in the combustor. Conventional scales of electric spark ignition mode are no longer suitable for micro combustion mode. The combustion is more unstable for the ignition and combustion quenching feature size is close to the size of combustor. Many efforts have been made to improve flame stability in microcombustors. Catalytic combustion is a way of stabilizing flame. Ran et al. [9-11] studied catalytic combustion of CH<sub>4</sub>/O<sub>2</sub> mixture in a micro-channel with the height of 1 mm and the length of 10 mm, the results manifested that fuels can combust at a low temperature when some catalysts were attached on the reaction surface. Zhong et al. [12,13] investigated the effects of wall condition, inlet velocity and the type of catalyst on the combustion characteristics and extinction limit in a micro-channel, which the diameter was 1 mm and the length of channel is 10 mm, the results



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confirmed that extinction was affected by the wall temperature and the catalyst covering rate. Yan et al. [14] had a research on the combustion characteristics of methane/air in micro-channel (20 mm  $\times$  $4 \text{ mm} \times 1 \text{ mm}$ , wall thickness of 0.2 mm) covered on Rh catalyst. It showed that adding hydrogen was benefit for methane combustion. Zhang et al. [15] investigated the characteristics of catalytic flow, combustion and heat transfer in micro-channel. The results showed that wall temperature had major influence on methane conversion. In addition, thermal managements, such as heat recirculation, is an excellent way to sustain stable flames. The Swiss-roll combustor has been studied as a favorable structure of heat recirculation and it had a positive effect on flame stabilization [16,17]. Fan et al. [18–22] developed micro-combustor with a bluff body which can absorb more high temperature gas and rise the combustion temperature. The height of the channel was 1 mm and the total length was 16 mm. They investigated the effect of bluff body shape on the extinction limit with a detailed hydrogen/air reaction mechanism, the results showed that the extinction limits for the triangular bluff body was smaller than the semicircular case. Li et al. [23] developed a micro-combustor, which had the size of 10 mm  $\times$  3 mm, with some stainless steel grids, the results demonstrated that the flame was anchored by adding the porous media. Nosrati et al. [24] analyzed micromixing for mixed electroosmotic or pressure driven flow of Newtonian fluid in micro-channels. The results showed that species mixing was improved by increasing the channel height but decreased with the increasing of Re number.

Concave cavity can increase the combustion efficiency and stability. Hence, the concave cavity technology is commonly used to increase the stability of supersonic combustion [25-27]. But the effect of concave cavity on the slow flow combustion is not further studied. Fan et al. studied the effects of concave cavity length to depth ratio, inlet velocity and equivalent ratio on the characteristic of hydrogen/air premixed gas phase combustion [28,29] in a micro-channel. The length of channel was 10 mm and the height was 1 mm. The cavity depth was 0.5 mm. The effect of convex cavity like fins on combustion characteristic is not commonly studied. Li et al. [30] studied methane/air combustion inside a microchannel (length of 10 mm, height of 0.6 mm, width of 5 mm) with fins. The simulation results showed that the axial fins had a strong influence on combustion and heat transfer. Li et al. [31,32] proposes a novel design concept for the enhancement of methane combustion in a micro-channel that uses the combined effects of catalyst segmentation and cavities. The reactor was 3 cm in length and had a wall thickness of 0.2 mm, the cavity width was 1 mm and the depth was 0.2 mm. The effects of a multi-segment catalyst and cavities on channel walls are examined and discussed in terms of various catalyst layouts, cavity dimensions, and flow conditions. There are not so many researches on the field of catalytic combustion in the micro-channel with cavity, but a similar channel model, like the constricted micro-channel, is used in many bio-fluid systems or fluidic devices without combustion. This kind of channel can enhance the rate of heat and mass transfer. Bigham and Shokouhmand et al. [33,34] studied the fluid flow and heat transfer through a constricted micro-channel. They mainly studied the effects of Knudsen number, viscous dissipation and geometry on the Re and Nusselt number on the undeveloped fluid flow. The results showed that Knudsen number has declining effect on both the Cf.Re and Nusselt number. Viscous dissipation can effect the thermal fluid pattern and increase the Nu. They [35] also studied slip-flow and heat transfer of gaseous flows in the inlet of a wavy micro-channel. The results indicated Kn also had a negative effect on Re and Nu. Viscous dissipation had a significant influence on Nu number. Above all, this channel model is available.

Stability of combustion also can be improved by using catalyst. With this consideration, the study of catalytic micro-combustor with a convex and concave cavity, respectively, is necessary. The catalytic combustion of methane/air at a low inlet velocity in concave and convex cavity micro channels, respectively, are numerically simulated. And the inner wall combustion characteristics of micro-combustor with and without a concave and convex cavity are developed and compared, and then the structure of the micro-combustor is optimized. A straight micro-channel is adopted for comparison as well.

#### 2. Numerical methods

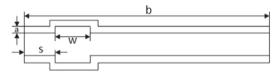
#### 2.1. Geometrical model

The schematic diagrams of the micro-channels with concave and convex cavity, respectively, are depicted in Fig. 1. The length of the micro-channel (b) is 10 mm. The height (c) is 1 mm and the wall thickness (a) is 0.2 mm. The distance from left side wall of the concave or convex cavity to the inlet side (s) is 1.2 mm, respectively. The depth (d) and length (w) of the concave cavity are 0.2 mm and 1.5 mm, respectively. The convex cavity has the equal size as the concave one but in opposite direction. A straight micro-channel (10 mm 1 length, 1 mm height, wall thickness of 2 mm) is studied for comparison.

#### 2.2. Grid method and boundary conditions

Different mesh size has been tested to ensure grid-independent. Quadrilateral mesh (0.03 mm) was adopted to channel dividing. Decreasing the mesh interval from 0.03 had no advantages, but also increased the computational difficulty and time. Thus, the micro-channel with concave cavity, the channel with convex cavity and the straight channel were composed by 15,730 meshes, 13,260 meshes and 14,586 meshes, respectively.

The computational fluid dynamics soft Fluent6.3 was applied to simulate the problem. The dimension of the micro-channel was small and the gas velocity was slow. The Reynolds number based on these parameters was very small, so laminar model was selected in this work. As for the boundary conditions, the velocity inlet and natural outflow were specified at the entrance and exit of the channel, respectively. The inlet temperature of mixture CH<sub>4</sub> and air was 573 K. Moreover, the inner wall surface was covered with Rh catalyst and the fluid–solid heat coupling was used in this work.



(a) Schematic diagram of micro-channel with concave cavity



(b) Schematic diagram of micro-channel with convex cavity



(c) Schematic diagram of straight micro-channel

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