FEDSM-ICNMM2010-' 00%+

NUMERICAL ANALYSIS OF CH4 AND AIR COMBUSTION INSIDE A SMALL TUBE WITH A TEMPERATURE GRADIENT

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ABSTRACT

A numerical study on CH₄ and air premixed combustion inside a small tube with a temperature gradient was undertaken to investigate the effects of inlet velocity, equivalence ratio and combustor size. The simulation results show that the inlet velocity has a significant influence on the reaction zone, and the flame front shifts downstream as the inlet velocity increases. The results also show that, the inlet velocity has no obvious effects on the flame temperature. The highest flame temperature is obtained if the equivalence ratio is set to 1. It is disclosed that the combustor size has a very strong effect on combustion characteristics. The smaller the combustor size is, the more difficult it is to maintain the steady combustion. The smallest combustor size that the stable flame can be sustained is determined mainly by the wall temperature of the microcombustor under the given conditions, and the higher the wall temperature is, the smaller the smallest combustor size. Therefore raising wall temperature is an effective way to realize flame stabilization for a given combustor size.

INTRODUCTION

The demand for miniaturized power source is increasing quickly as the fast development of MEMS devices. A key component of these devices is a micro-combustor in which the fuel-air mixture is burnt.^[1] Micro-combustors using hydrocarbons as fuel may play a vital role in the portable production of energy, because hydrocarbons have an energy density significantly larger than that of the traditional Li batteries.^[2] Compared with the traditional combustors, combustion in micro-combustors becomes less efficient due to the intensified heat loss from the flame to the combustor wall,

NOMENCLATURE

- *D* diameter of the tube combustor, m
- f Equivalence ratio, -
- *L* length of the tube combustor, m
- *r* radial coordinate, m
- *T* temperature, K
- *x* axial coordinate from the inlet, m

radical destruction at the gas-wall interface and reduced residence time. The combustion process inside microcombustors are different from that of the conventional scale and insufficient in fundamental knowledge related to microcombustion.^[3]

Norton and Vlachos^[4] simulated CH₄ and air premixed combustion in a 2D rectangle combustor and analyzed the influences of the size of the gap between the walls, wall thickness, thermal conductivity of wall material and the heat transfer coefficients on the combustion characteristics. Kaisare et al.^[5] analyzed the influence of the 2D rectangle combustor length, the size of the gap between the wall and wall thickness on distinction limits and gave the optimized gap size for the flame stabilization. Maruta et al.^[6] did experimental studies to investigate the characteristics of premixed combustion in a small tube with a temperature gradient, they found that stable flame branches in high and low mixture velocities, and in the intermediate mixture velocities repetition of extinction and ignition, and pulsating flames were observed. Hua et al.^[7] carried out a numerical study of CH₄ and air combustion in micro-tubes with different diameters and stressed on the influences of different heat transfer conditions and wall thermal conductivities. The numerical and experimental investigations related to the combustion in a narrow tube with a temperature

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gradient are quite limited though the situation is very common in practical small scale combustors.

The present study concerns the combustion characteristics of CH_4 and air mixture inside a small diameter tube with a temperature gradient, and the influences of inlet velocity, equivalence ratio and combustor sizes are analyzed.

THE MODEL

The combustor is a circular tube with a diameter of D and a length of L, as shown in Fig. 1. It is assumed that the fuel and air is fully mixed before they flow into the combustor, and the

second-order up-winding method is used to discretize the governing equations and SIMPLE algorithm is used to decouple the pressure-velocity coupling. Computations were performed using meshes with varying nodal densities to determine the optimal node spacing and density that would give the desired accuracy and minimize the computation time. Finally we chose a mesh with 1500 uniform nodes.

RESULTS AND DISCUSSION

Effects of velocity



Fig. 1 Geometry model

heat transfer between the wall and the environment is constant and uniform over the whole external wall surface of the tube. Dufour and gas radiation effects are simply neglected and work done by pressure and viscous forces is not taken into consideration. Also the system has experienced long time running and the steady state is acquired. With these assumptions, the problem is simplified into a 2D axial symmetric problem. The heat conduction in the wall was not taken into consideration, and a non-uniform temperature distribution along the wall used here is from [6] and is fitted by the following equation,

$$T = 1267.722 - \frac{985.571}{1 + \exp\left(\frac{x + 5.512}{4.804}\right)}$$
(1)

Note that the inlet of the combustor is not set at x= 0. The governing equations of continuity, momentum, spec ies and energy for gas phases can be found elsewhere.^[7]

To analyze the influence of the inlet velocity, the mixture velocity varied from 0.3 m/s~1.5 m/s, the equivalence ratio varied from 0.85~1.2 and the diameter of the combustor varied from 1.0 mm~2.0 mm. FLUENT 6.2 is used to carry out the global numerical computations. One-step reaction mechanism^[7] is used for CH_4 and air combustion. At the inlet a fixed flat velocity profile is assumed and at the exit, a fixed pressure is imposed for the rest of the variables. To solve the governing equations, a segregated solution solver with an under relaxation method is used, the segregated solver first solve momentum equations and then continuity equation and updates pressure and mass flow rate. The energy and species equations subsequently solved and convergence is checked. The gas density is calculated using the ideal gas law. The gas viscosity, specific heat and thermal conductivity are calculated as a mass fraction-weighted average of all species. The specific heat is calculated using a piecewise polynomial fit of temperature.^[8] A

The effects of inlet velocity of the methane-air mixture on the flame temperature along the axis of the combustor (r=0) is shown in Fig. 2. The inlet of the micro-combustor is located at x=-0.03m and the outlet is located at x=0.04m. From this figure, one can see that as the inlet velocity increases, the



Fig.2 Influence of inlet velocity on temperature distribution along the axis (f=1.0)

location of the peak value of the flame temperature at the axis of the combustor or the flame front is shifted downstream. The peak flame temperature first increases with the inlet velocity to a certain value for small inlet velocities and then, after the inlet velocity exceeds a certain critical value (e.g. ≥ 0.8 m/s), this peak temperature remains a constant and is independent of the inlet velocity. These results show that as the velocity increases, the main reaction zone shifts downstream. With the existence of the wall temperature gradient, at relatively low inlet

velocities (e.g. ≤ 0.8 m/s) the flame location is in front of the highest wall temperature zone. Due to the relatively weak convective heat transfer and the smaller temperature difference between the methane-air mixture and the wall, the mixture is not fully preheated before combustion is completely actuated, and this will certainly leave to a relatively low flame temperature. As the inlet velocity increases, the main reaction zone shifts down stream. The convective heat transfer and the temperature difference between the methane-air mixture and



Fig.3 Influence of inlet velocity on mass fraction distribution of CH_4 along the axis (*f*=1.0)



Fig.4 Influence of equivalence ratio on temperature distribution along the axis

the wall are enlarged; the mixture is thus well preheated, so the

flame temperature increases with the inlet velocity. However, as the velocity exceeds a certain value (e.g. 0.8m/s), the flame front is shifted further to the downstream, the convection heat transfer coefficient and the temperature difference between the wall and the methane-air mixture acquire their maximum values for the given thermal boundary conditions. The mixture is thus preheated to its highest possible temperature, and therefore the peak flame temperature reaches to its highest value for the given thermal conditions. After this, although the reaction zone shifts downstream as the velocity increases, the peak flame temperature remains its highest value and is independent of the inlet velocity. These results also show that the heat transfer condition between the methane-air mixture and the wall may strongly influence the characteristics of combustion. The influence of the inlet velocity on the mass fraction of CH₄ along the axis is shown in Fig. 3. For relatively low inlet velocities, CH₄ is burned out within a very narrow zone. The reaction zone increases with the inlet velocity due to the intensified mass transfer along the axis which makes CH₄



Fig.5 Influence of combustor size on temperature distribution along the axis

diffuse further downstream.

Effects of equivalence ratio

In order to analyze the influences of the equivalence ratio on the combustion characteristics, simulations are performed for inlet velocity of 0.5m/s and a 2mm-in-diameter combustor over a wide range of equivalence ratio. Some of the typical results are depicted in Fig. 4 with equivalence ratios equal to 0.85, 1.0 and 1.2, respectively. From this figure, we can see that the peak flame temperatures of the equivalence ratios equal to 0.85 and 1.2 are lower than that of the equivalence ratio equal to 1.0. From the definition of equivalence ratio, the equivalence ratio equals to 0.85 means that CH_4 is insufficient and less fuel is provided than that of the stoichiometric combustion (equivalence ratio equals to 1), the peak flame temperature is therefore lower than that of the stoichiometric combustion. On the other hand, if the equivalence ratio is larger than 1, the CH_4 is excessive, and less air (and thus oxygen) is provided due to the fixed inlet velocity. Therefore, the CH_4 that is consumed per unit time is also less than that of the stoichiometric combustion (equivalence ratio equals 1), so the peak flame temperature is also lower. Actually, even if the CH_4 consumed per unit time is same, the peak flame temperature of the non-stoichiometric combustion (equivalence ratio is not equal to 1) is still lower than that of the stoichiometric combustion (equivalence ratio equals 1), because the heat of combustion will either heat the excessive CH_4 or air.

Effects of combustor size

Combustor is in reality three dimensional. However, for the geometry given here, the size that dominates the combustion inside the combustor is its diameter according to heat, mass transfer and combustion theory. Therefore, here discussions are limited to the influences of the combustor tube diameter on the combustion characteristics. In order to analyze the influence of the combustor size on the characteristics of combustion, simulations are performed for inlet velocity of 0.5m/s and the equivalence ratio of 0.85 over a wide range of the combustor tube diameters. Fig. 5 presents some of the typical simulation results of the axial temperatures distributions for three different combustor tube diameters. The numerical simulation results show that the combustor size has very significant influences on the combustion characteristics. Steady combustion can be achieved in the combustors with a diameter of 2.0mm and 1.5mm, respectively. And the axial temperature distribution shows no obvious changes in the case of the 1.0mm-in-diamter combustor, which means that no combustion occurs under the given thermal conditions. Besides the velocity and equivalence ratio, the wall temperature also affects the combustion characteristics. If the wall temperature of the combustor tube with a diameter of 1.0mm is elevated to a higher value, then combustion may be initiated and a steady combustion inside the combustor may be maintained as well. If the maximum value of the wall temperature is changed from 1270K to 1470K in Eq. (1), then a steady combustion does appear in the 1mm-indiameter combustor as expected, as shown in Fig. 6. The simulations are also carried for the maximum value of the wall temperature in Eq. (1) is set to 1370K, 1420K and 1450K. For these lower wall temperature situations, only partial oxidation reaction is observed. Therefore, the temperature with the maximum wall temperature value in Eq. (1) is the lowest temperature for the 1mm-in-diameter combustor to maintain steady combustion under the given flow and combustion conditions (inlet velocity, 0.5m/s; equivalence ratio, 0.85). Furthermore, as one may understand, the inlet velocity of the methane-air mixture should also influence the lowest wall temperature distribution. The simulations were repeated for the situation that the inlet velocity is set to 1.0m/s. The results show that the lowest temperature profile for the 1mm-indiameter combustor to maintain steady combustion in this case is that with the maximum wall temperature value set to 1420K in Eq. (1), as shown in Fig. 7. Comparing with the results of the



Fig.6 Influence of wall temperature on temperature distribution along the axis

inlet velocity of 0.5m/s, we find that the higher inlet velocity results in a lower wall temperature to maintain steady combustion. This is because the high velocity enhances the preheating effect on the methane-air mixture and this is in accordance with the previous discussions about the influences of inlet velocity. These results show that the smallest combustor size that steady combustion can occur is determined by the inlet



Fig.7 Influence of wall temperature on temperature along the axis at higher velocities

velocity, wall temperature, and of course equivalence ratio.

CONCLUSIONS

The premixed combustion of CH_4 and air in a small tube with a temperature gradient is numerically investigated, the effects of inlet velocity, equivalence ratio and combustor size are discussed in this paper. From the above discussions, the main conclusions are summarized as follows:

(1) The inlet velocity has a strong effect on combustion zone. The combustion zone shifts down stream as inlet velocity increases, but it has no obvious effects on flame temperature;

(2) The equivalence ratio is a key parameter that affects the combustion characteristics. The highest flame temperature is obtained if the equivalence ratio is set at 1;

(3) The combustor size shows a very strong influence on combustion characteristics. The smaller the combustor size is, the more difficult it is to maintain the steady combustion. The smallest combustor size that the stable flame can be sustained is determined mainly by the wall temperature of the combustor tube and the inlet velocity, and the higher the wall temperature is, the smaller the smallest combustor size. Therefore raising wall temperature is an effective way to realize flame stabilization for a given combustor size.

REFERENCES

 Chemical Engineering Journal, 150, 213-222, 2009 -A numerical study on premixed micro-combustion of CH4–air mixture: Effects of combustor size, geometry and boundary conditions on flame temperature, J. Li, S. K. Chou, W. M. Yang, Z. W. Li.

- [2] The Third Asia–Pacific Conference on Combustion, Seoul, Korea, 2001-Combustion in microscale heat-recirculating burners, L. Sitzki, K. Borer, E. Schuster, P. D. Ronney, S. Wussow
- [3] **Proceedings of the Combustion Institute, 29, 883– 898, 2002** - Micropower generation using combustion: issues and approaches, A. C. Fernandez-Pello
- [4] **Chemical Engineering Science**, **58: 4871-4882, 2003** -Combustion characteristics and flame stability at the microscale: a CFD study of premixed methane/air mixtures, D. G. Norton, D. G. Vlachos
- [5] **Catal. Today, 120, 96-106, 2007 -** Optimal reactor dimensions for homogeneous combustion in small channels, N. S. Kaisare, D. G. Vlachos
- [6] Proceedings of the Combustion Institute, 31, 2429 -2436, 2005 - Characteristics of combustion in a narrow channel with a temperature gradient, K. Maruta, T. Kataoka, N. I. Kim, S. Minaev, R. Fursenko
- [7] An Introduction to Combustion-Concepts and Applications, International Editions 2000, McGraw-Hill Book Co – Singapore, 2000, S. R. Turns
- [8] Chemical Engineering Science, 60:3497-3506, 2005 -Numerical simulation of the combustion of hydrogen-air mixture in micro-scaled chambers. Part I. Fundamental study, J. S. Hua, M. Wu, K. Kumar