A CFD Study of Dimensional Scaling effect on the Combustion of Hydrogen-Air Mixture in Micro-Scale Chambers with Same Shape Aspect Ratio

R.KAMALI , A.R.BINESH
Department of Mechanical Engineering
Shiraz University
Zand Street, School of Engineering, Shiraz University, Shiraz
IRAN

Abstract: - Understanding of the flow dynamics, chemical kinetics and heat transfer mechanism within micro-combustors is essential for the development of combustion-based power MEMS devices, which may supply much higher energy density than the batteries used nowadays. In the present work, a computer code has been developed to study the combustion of hydrogen–air mixture in a series of chambers with same shape aspect ratio but various dimensions from millimeter to micrometer level. The prepared algorithm and the computer code are capable of modeling mixture effects in different fluid flows including chemical reactions, viscous and mass diffusion effects. The transition of the combustion phenomena in the chambers from relatively large scale to micro-scale has been studied numerically to investigate the micro-combustion mechanism. The simulation results under the adiabatic wall condition indicate that the decreasing of combustion chamber size does not have significant effect on the global chemical reaction rate within the chamber, but it may limit the combustion efficiency. Through such systematic numerical analysis, a proper operation space for the micro-combustor is suggested, which may be used as the guideline for micro-combustor design. In addition, the results reported in this paper illustrate that the numerical simulation can be one of the most powerful and beneficial tools for the micro-combustor design, optimization and performance analysis.

Key-words: - Numerical simulation, Micro-combustion, MEMS, CFD, Chemical reaction

1   Introduction

With the rapid progress in the mobile electrical and micro devices such as micro actuators, sensor, air vehicle and robots in the recent years, the demands on the micro-power supplier with high power density is increasing, and fabrication of such micro-devices is becoming possible. The batteries used nowadays have quite low specific energy (0.6 kJ/g for an alkaline battery and 1.2 kJ/g for a lithium battery) compared to hydrogen (140 kJ/g) and hydrocarbon fuels [2]. The combustion-based micro-power device, such as micro-gas turbine engine, is one of the most promising designs due to its high power density. Development of miniaturized combustion-based power generating devices, even with a relatively inefficient conversion of hydrogen fuel to power, would result in increased lifetime and/or reduced weight of an electronic or mechanical system that currently uses batteries for power. Recent advances in the field of silicon micro-fabrication techniques and silicon-based Micro-Electro-Mechanical Systems (MEMS) have led to the possibility of a new generation of micro heat engines for power generation. Micro-combustor is one of the critical components for micro-power system using hydrogen and hydrocarbon fuels as an energy source. Several types of micro-combustor and chemical reactor are currently under development [1]. However, as the size of micro-combustion chamber decreases to micron level, which is comparable to the laminar flame thickness, traditional combustion theory may not be able to explain and predict the details about the micro-combustion phenomena within the micro-combustor. In addition, the experimental method and diagnostic techniques developed for the macro-combustion facilities, becomes inapplicable for the micro-combustor due to the limitation of combustion chamber size and the complexity of the micro-combustion physics. Hence, development of a new cost-effective analyzing tool for micro-combustor system is essential to understand the details about the fluid dynamics, chemical kinetics and heat transfers occurring in micro-combustor, bridging

the fundamental knowledge, experimental measurement and engineering design and optimization.

The past experimental works [2] have proved that it is impossible to propagate flames in a small gap around millimeter scale, which is known as quenching distance. The investigation indicates that there are two kinds of mechanisms, namely thermal quenching and radical quenching, leading to flame quenching in smaller dimension [3]. Some theoretical analysis of the combustion mechanism in simple micro-chambers has been performed [4] to show the feasibility of stable combustion in micro-combustor. The fundamental understanding of combustion mechanism in micro-scaled chambers, which is very essential to the design and optimization of power MEMS devices, is not understood well at present. Due to the difficulties in conducting spatially resolved measurements of combustion characteristics in micro-scale devices, the numerical simulation can be a cost-effective approach to study the micro-combustion mechanism. Norton and Vlachos [5] conducted two-dimensional CFD simulation to analysis the premixed methane/air flames stability in a micro-combustor, consisting of two parallel, infinitely wide plates of length of 1 cm and small distance. Norton and Vlachos [6] reported the CFD study on the micro-combustion stability of propane/air mixture. Choi [7] performed the numerical simulation of hydrogen/air flame propagation near extinction condition in a micro-combustor. Spadaccini [8] studied the temperature distribution within combustion chamber with different inlet geometries using three-dimensional numerical simulation accounting the chemical kinetics hydrogen–air reaction mechanism. In this paper, Computational Fluid Dynamics (CFD) - based numerical simulations are conducted to study the combustion of stoichiometric hydrogen–air in a number of micro-scaled cylindrical chambers. Detailed chemical reaction mechanism in combustion of hydrogen–air mixture is employed in the CFD simulations. In order to study the dimensional scaling effect on the combustion, the aspect ratio of the combustion chamber is kept the same in all simulations.The chamber dimension, e.g. inlet diameter of chamber, is scaled down from millimeter level to micron level. The simulation results indicate that stable combustion in a micro-scaled chamber can be achieved through balancing the flow residence time and the chemical reaction time and optimizing the thermal condition. Since the residence time will be shortened in a micro-combustion chamber, it is important to shorten chemical reaction time as well in order to ensure the completion of the combustion process. According to the chemical kinetics theory, one of the possible measures to shorten the chemical reaction time is to increase the reaction rate by ensuring a high reaction temperature. This in turn can be achieved by reducing the heat loss from the combustion chamber.

2 Computational model

2.1 Model geometry and the mesh

The geometry of the cylindrical chamber used in this study is shown in Fig. 1. The effects of chamber dimension on combustion characteristics are studied through scaling down the cylindrical chamber from a relatively large scale to a micro-scale while keeping the same shape aspect ratio. The inlet diameter (D) of the chamber is varied from the large size to the small size at 0.5, 0.2, 0.08, and 0.045 mm, respectively. The ratio of chamber diameter to inlet diameter (D) is maintained at 2. The ratio of chamber length (L) to inlet diameter (D) is fixed to be 10. Stoichiometric hydrogen–air mixture is injected into the cylindrical chamber from the inlet located at one axial end with a step expansion as shown in Fig. 1. Because of the axial symmetry of the combustion chamber, the geometry is modeled as a two-dimensional axi-symmetric model. For the all cases analyzed in this study, a structured grid is used to mesh the models for the CFD simulations as shown in Fig. 2. The whole computational domain including both combustion chamber and inlet throttle is meshed using about 24375 cells. This fine mesh size will be able to provide good spatial resolution for the distribution of most variables within the combustion chamber.
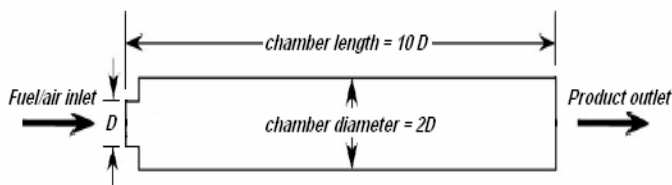

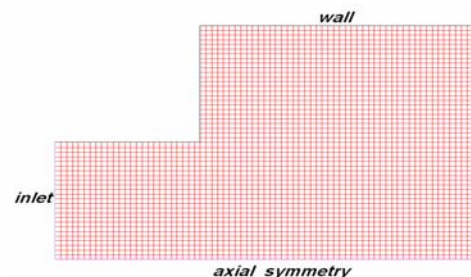Fig. 1. Schematic diagram of the micro-scaled combustion chamber for micro-combustion modeling.

Fig. 2. Numerical grid of the computational domain at inlet

2.2 Fluid flow modeling

The characteristic length of the combustion chamber and the reacting gas flow path in micro-combustors, even for MEMS systems, is still sufficiently larger than the molecular mean-free path (average distance between two successive collisions of a molecule) of the air and other gases flowing through the systems. Hence, the fluid media can be reasonably considered as continuum in this study. The Navier–Stokes equation is solved using eulerian mixture model for the fluid domain and no-slip condition on the wall is applied.

2.3 Governing equations

A computer code is used to perform numerical simulations of the fluid flow in combustion chamber by solving the conservation equations of mass, momentum, energy and species.

Continuity Equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0 \tag{1}$$

Momentum Equation:

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \tag{2}$$

Where the stress tensor τ_{ij} is given by

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\mu\delta_{ij} \, divV \tag{3}$$

Where μ is the molecular viscosity and the second term on the right hand side is the effect of volume dilation.

Energy Equation :

$$\frac{\partial}{\partial t}(\rho E) + \frac{\partial}{\partial x_i}(u_i(\rho E + p)) =$$

$$\frac{\partial}{\partial x_i}\left(k_{eff}\frac{\partial T}{\partial x_i} - \sum_j h_j J_j + u_j(\tau_{ij})_{eff}\right) + S_h \tag{4}$$

Where k_{eff} is the effective conductivity and J_j is the diffusion flux of species j. The first three terms on the right-hand side of Equation   represent energy transfer due to conduction, species diffusion, and viscous dissipation, respectively. S_h includes the heat of chemical reaction, and any other volumetric heat sources we have defined. In equation (4),

$$E = h - \frac{P}{\rho} + \frac{u_i^2}{2} \tag{5}$$

where sensible enthalpy h is defined for ideal gases as

$$h = \sum_j m_j h_j \tag{6}$$

Where m_j is the mass fraction of species j.

Species Conservation Equation:

When we choose to solve conservation equations for chemical species, we predicts the local mass fraction of each species, m_i, through the solution of a convection-diffusion equation for the i th species. This conservation equation takes the following general form:

$$\frac{\partial p}{\partial t}(\rho m_i) + \frac{\partial}{\partial x_i}(\rho u_i m_i) = -\frac{\partial}{\partial x_i}J_{i,i} + R_i + S_i \tag{7}$$

where R_i is the net rate of production of species i by chemical reaction and S_i is the rate of creation by addition from the dispersed phase. An equation of this form will be solved for $N-1$ species where N is the total number of fluid phase chemical species present in the system. Since the mass fraction of the species must sum to unity, the N th mass fraction is determined as one minus the sum of the $N-1$ solved mass fractions. To minimize numerical error, the N th species should be selected as that species with the overall largest mass fraction, such as N_2 when the oxidizer is air. $J_{i,i}$ is the diffusion flux of species i, which arises due to concentration gradients. We use the dilute approximation, under which the diffusion flux can be written as

$$J_{i,i} = -\rho D_{i,m}\frac{\partial m_i}{\partial x_i} \tag{8}$$

Here $D_{i,m}$ is the diffusion coefficient for species i in the mixture. The reaction rates that appear as source terms in Equation (8) are computed by Laminar finite-rate model that effect of turbulent fluctuations are ignored, and reaction rates are determined by Arrhenius expressions. The net source of chemical species i due to reaction R_i is computed as the sum of the Arrhenius reaction sources over the N_R reactions that the species participate in:

$$R_i = M_i \sum_{k=1}^{N_R} \hat{R}_{i,k} \tag{9}$$

where M_i is the molecular weight of species i and $\hat{R}_{i,k}$ is the Arrhenius molar rate of creation/destruction of species i in reaction r.

2.4 Boundary conditions

A fixed composition (a stoichiometric mixture) of hydrogen–air is specified at the fuel inlet of micro-combustion chamber. The inlet temperature of fuel mixture is considered to be uniform at 300 K. A fixed,

uniform velocity 5 m/s is specified at the inlet. As the combustion chamber diameter is about twice of the diameter inlet of fuel/air mixture. Hence, the cross-section area of the combustion chamber will be about four times of the inlet area. The averaged velocity of gas mixture at the chamber cross section will be about 1.25 m/s before it is burnt. Since the averaged gas mixture velocity of 1.25 m/s is lower than the flame speed, it will help the flame stable in the combustion chamber. Axi-symmetric boundary conditions are applied along the central axis of the combustion chamber. At the exit, a pressure outlet boundary condition is specified with a fixed pressure of 1.013×10^5 Pa. At the chamber wall, no-slip boundary condition and no species flux normal to the wall surface are applied.

2.5 Numerical model

A segregated solution solver is used to solve the above-mentioned set of governing equations. Since the Reynolds number of the fluid flow ranges from about 11 when D=0.045mm to 126 when D=0.5mm for the simulated cases, laminar viscous flow is considered. The fluid density is calculated using the ideal gas law. The fluid mixture specific heat, viscosity, and thermal conductivity are calculated from a mass fraction weighted average of species properties. The combustion model is validated by simulating the combustion of premixed hydrogen–air under adiabatic condition and comparing with the measurement of adiabatic flame reported by Glassman [3]. The comparisons of flame temperature and mole fraction of species obtained from the model prediction and experiment are listed in Table 1. The numerical predictions are in reasonable agreement with the experimental data.

Mole fractions	Experimental results (Glassman, 1996)	Numerical results
H_2O	0.323	0.335
O_2	0.005	0.008
H_2	0.015	0.011
N_2	0.644	0.644
NO	0.003	0.002

Table 1. Comparison of mole fraction of species in stoichiometric hydrogen–air mixtures in simulation and experiment

3   Results and discussion

A number of numerical simulations have been performed to study the combustion phenomena when the combustion chamber size is reduced from a relatively large scale to a micro-scale under adiabatic wall condition. Fig. 3 shows the predicted temperature contours on the cross section of combustion chambers

for different inlet diameters: (a) 0.5 mm, (b) 0.2 mm, (c) 0.08mm and   (d) 0.045 mm, under adiabatic wall condition. For the same simulation cases, the contours of Arrhenius rate of reaction, which is regarded as an indicator of global chemical reaction rate, are shown in Fig. 3. The combustion chamber dimensions shown in these contour plot figures are normalized by the corresponding inlet diameter (D) for each simulation case. In this way, the relative position of combustion zone and physical property distribution in the different-sized combustion chambers can be easily compared.

It can be seen from Figs. 3 and 4 that the combustion can be self-sustained in the micro-scaled combustion chamber if the wall is maintained as adiabatic. The gas temperature is raised significantly due to the heat released from combustion. The highest temperature is obtained at the exit of combustion chamber at a range of 2600–3000 K. The flame temperature can be as high as 3000K for the largest combustor in this study, which is almost the same as the adiabatic flame temperature of the combustion of stoichiometric hydrogen–air mixture. As the combustion chamber size decreases, the exit temperature of the combustion product decreases as well. However, as the combustion chamber size decreases, the ratio of the combustion zone to chamber volume increases significantly as shown in Fig. 3.

Figs. 5–7 show the gas temperature, Arrhenius rate of reaction and hydrogen conversion rate distributions along the central axis of the chamber, respectively. Here, the hydrogen conversion rate is defined as $([H2]_{initial} - [H2])/[H2]_{initial}$ and   the dimensionless axial distance is defined as the ratio of the axial distance to the inlet diameter.
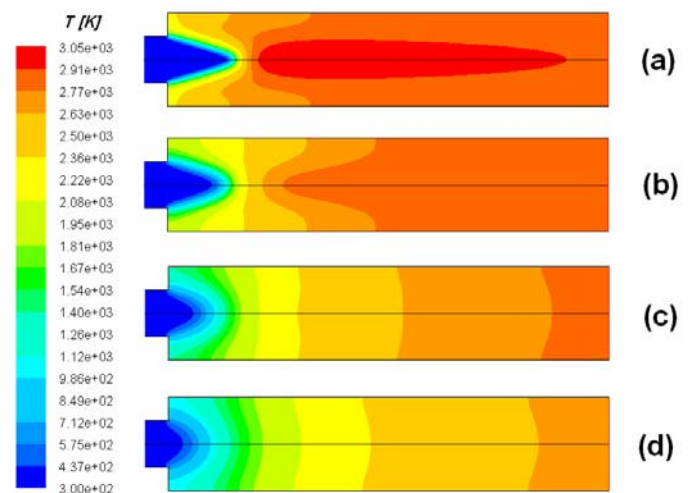

Fig. 3. Contours of temperature [K] on the cross section along central axis of various sized combustion chambers with the inlet diameter of: (a) 0.5 mm; (b) 0.2 mm; (c) 0.08 mm; (d) 0.045mm under adiabatic wall condition.
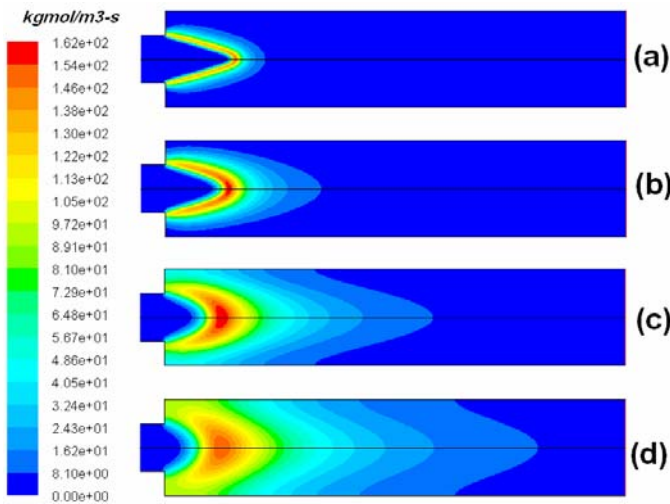
Fig. 4. Contours of production rate [kgmol/m3-s] of water at the cross section along the central axis of various sized combustion chambers with the inlet diameter of: (a) 0.5 mm; (b) 0.2 mm; (c) 0.08 mm; (d) 0.045mm under adiabatic wall condition.
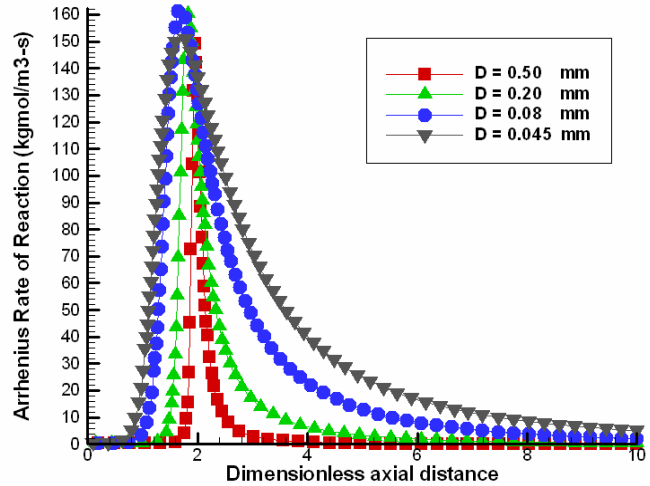

Fig. 6. Water production rate [kgmol/m3-s] distribution along the central axis for the scaled chambers of various inlet diameters (D) under adiabatic wall condition.
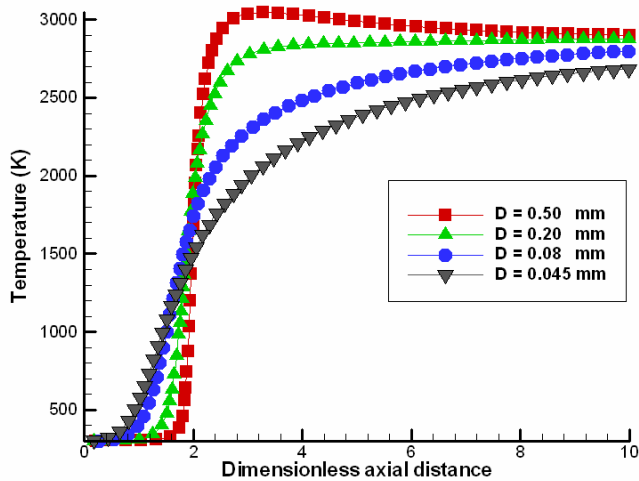

Fig. 5. Gas temperature [K] distribution along the central axis for the scaled chambers of various inlet diameters (D) under adiabatic wall condition.
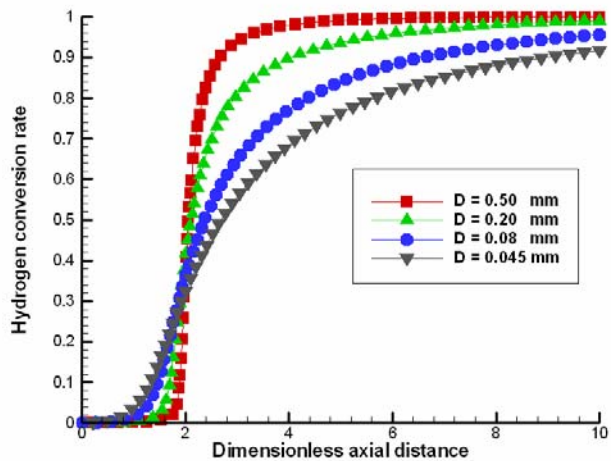

Fig. 7. Distribution of hydrogen conversion rate along the central axis for the scaled chambers of various inlet diameters (D) under adiabatic wall condition.

When the chamber dimension is large enough, the gas mixture has enough residence time in the chamber, so that combustion will be completed before it flows out of the combustion chamber. Hence, it can be seen in Fig. 5 that a narrow peak is formed for the large chambers due to the reaction confined to a narrow zone. With the completed combustion in the large chambers, the gas product flows out of the combustion chamber almost at adiabatic flame temperature 3000K as n Fig. 5. However, when combustion chamber size decreases, the chemical reaction mechanism is kept same. The reaction zone may occupy more and more space of the micro-combustion chamber. Hence, it can be seen from Fig.6

that the peak of Arrhenius rate of reaction becomes wider as the chamber size decreases. Fig. 5 also indicates the temperature of the combustion gas product decreases as the combustion chamber size decreases due to the incomplete combustion in smaller chambers. The hydrogen conversion rate distributions shown in Fig. 7 indicate the smaller combustion chamber has higher conversion rate near the inlet, but lower conversation rate near outlet. It can be noted from Figs. 4 and 6 that the maximum water production rate maintain almost at the same level when the chamber dimension decreases, which means the chemical reaction rate does not change significantly as the combustion chamber size decreases.

The simulation results under the adiabatic wall condition indicate that the decreasing of combustion chamber size does not have significant effect on the global chemical reaction rate within the chamber. But, decreasing the combustion chamber size may limit the combustion efficiency. This is due to the fact that the gas mixture does not have enough residence time to finish the chemical reaction completely in the smaller chambers. Hence, to obtain a stable combustion in a micro chamber, the chamber dimension should be larger than the adiabatic flame thickness at least.

4 Conclusions

In the present work, a computer code has been developed to study the combustion phenomena of the hydrogen–air mixture in a series of combustion chambers when the inlet diameter is reduced from a relatively large size of 0.5mm to a micro-scale size of 0.045 mm.

The prepared algorithm and the computer code are capable of modeling mixture effects in different fluid flows including chemical reactions, viscous and mass diffusion effects.

Theoretically, stable combustion can only occur in a combustion chamber when the reactant residence time is larger than the chemical reaction time. For the case of combustion in traditional large-scale combustors, the residence time for reactant in the combustion chamber is always large enough for complete combustion. Decreasing the dimension of combustion chamber leads to significant reduction in residence time as the reactant flow speed cannot reduce accordingly. This is because a certain flow rate of reactant needs to be maintained to achieve the requirement of power generation rate. But, the chemical reaction time is remained as usual. The direct consequence of insufficient residence time in micro-combustion chamber is that the combustion may not be complete within the combustor. Lower combustion efficiency may lead to insufficient heat generation to maintain self-sustained combustion, and further result in quenching. The numerical simulation of combustion of premixed hydrogen–air in micro-scaled chamber with adiabatic wall condition proves that the combustion may be stable only when the combustion chamber size is large enough comparing to the adiabatic flame thickness.

Through numerical simulation of combustion of hydrogen–air mixture in micro-scaled chambers, it can be concluded that the numerical model is able to capture the basic micro-combustion mechanism. The quenching phenomena and mechanism in micro-combustion have been explored and discussed. Stable combustion in the micro-combustor is achievable by system optimization of the combustor geometry, thermal conditions and reacting flow dynamics. The numerical modeling approach presented in this paper is helpful in the design and optimization of combustion-based micro-power generation device.

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