NUMERICAL STUDY OF THE EFFECTS OF HEAT TRANSFER METHODS ON CH_4/(CH_4+H_2)-AIR PREMIXED FLAMES IN A MICRO-STEPPED TUBE

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Abstract

In this study, an approach to modification and improvement of CH_4/air pre-mixed flame in a micro-stepped tube is studied numerically. The effects of added hydrogen to methane as an additive and some physical properties such as the micro-stepped tube wall thermal conductivity (K_w) and the outer wall convective (h_{out}) and radiative (e) heat transfer coefficients on temperature distribution and combustion progress in a micro-stepped tube are calculated using a high order, high accuracy 2D numerical laminar steady state code. The results show that adding hydrogen to methane in a micro-stepped tube can play a pivotal role in modification processes of combustion phenomena in a micro combustor. As compared to single back ward facing step method and also according to the wall thermal conductivity (K_w), hydrogen addition method can improve flame location inside the micro-tube 35% to 55% and increase uniformity of temperature distribution on the micro-tube wall. Also, it is found that adding hydrogen to CH_4 can assure the flame presence in some certain conditions in comparison to the simple backward facing step method. Moreover, the results indicate that the outer wall conductivity and emissivity have destructive effect on the flame properties inside the micro-combustor, so that they can decrease active radicals' concentration in combustion zone and combustor, impressively.

Introduction

Regarding the recent advances in semi-conductors and micro machining technologies by production feasibility of micro devices and rapid progress in this field, the demand for micro electrical and mechanical systems (MEMS) such as micro power generation and micro aerospace systems is increasing rapidly.

Regarding this growing demand, finding one suitable and appropriate energy resource for providing adequate energy for these types of mechanical devices still seems to be one of the main obstacles of the progress and advancement in this field of technology [1]. This matter can be so visible while MEMS device weight is very critical. Due to low ratio of weight to energy density of on hand productive resources of electrical power such as chemical batteries, application of these types of power generators sounds to be inapplicable in weight restricted MEMS devices. According to high ratio of volume to energy density, competitive cost and availability of hydrocarbon fuels, application of hydrocarbon fuels as energy source for MEMS devices even with low combustion efficiency still seems to be most suitable as one of the best sources of power generation in micro power generators as compared to the last technologies of batteries. Therefore, in recent years, application of hydrocarbon fuels as one of the appropriate source of power generation in micro power generators has been considered seriously.

Because of high surface to volume ratio in these kinds of combustion systems that typically reaches to about 2000 for a micro tube with 1 mm in radius, thermal and radical quenching and heat loss to ambient in micro combustors are much more dominant in comparison to meso or macro combustors. Thermal and radical quenching can effectively influence combustion process in these kinds of combustion chambers and may lead combustion process to quenching or blow out [2]. Therefore, in recent years, most experimental and numerical researches which are performed in micro combustion systems field have been focused on these topics, especially heat transfer process.

Since 2001 up to now, many experimental and numerical investigations into combustion process in micro-combustors, especially micro-tube and micro-channel have been accomplished by various researchers. Regarding these researches, it can be inferred that the micro combustor geometry such as wall thickness, inner diameter or height, heat transfer surface and inserting backward facing-step plays a crucial role in establishing a stable and efficient combustion in a micro combustor. This importance is due to several attributed reasons such as heat loss variations, heat transfer from post-flame zone to pre-flame region [3-5], the increment of reactive mixture residence time [6] and enhancement of mixing process [7], respectively. Also, some physical and chemical properties of micro-combustor wall and the inlet mixture such as fuel type [8], wall thermal conductivity [8-10], equivalence ratio and inlet velocity to combustion chamber can influence combustion process in a micro combustor, so that variation of wall thermal conductivity and its physical properties can govern the combustion procedures by proper preheating of fresh incoming mixture [9] or thermal and radical species quenching processes [11]. Furthermore, according to [12-16], unsteady and oscillatory operations are seen in certain conditions. Norton and Vlachos [8] proved that oscillatory behaviors occur near extinction limits. Regarding Maruta et al. [14] research, stable or oscillatory behavior of a micro-flame depends on various parameters such as equivalence ratio, inlet mixture velocity, micro-combustor geometry, outer wall heat transfer conditions [12], the micro-tube wall temperature and incoming mixture composition. Maruta et al. [14] and Minaev et al. [16] maintained that the instability occurs at moderate velocities and high or low enough incoming mixture velocities are located within stable combustion zones. As it is known, hydrogen addition into the conventional combustion systems which use hydrocarbon fuels as a prevalent fuel can improve combustion characteristics dramatically. Therefore, in another investigation performed by Zhang et al. [17], it is experimentally confirmed that adding hydrogen to methane as an additive fuel can facilitate ignition commencement and also expand the amplitude of methane stable combustion domain in a micro tube combustor.

Regarding literature review discussed above, at the present study, hydrogen addition approach to modification of CH_4/air pre-mixed flame in a micro-tube combustor is studied numerically. This approach has been studied at this paper due to importance of using hydrogen as a high quality, clean and on hand resource of energy for the next years. Moreover, it should be noticed that due to complexity of using hydrogen as a conventional fuel, blending usage of hydrogen with other hydrocarbons such as methane, propane and so forth can be counted as a remedy for increasing the efficiency of commercial hydrocarbons and also compensation of the complexity of hydrogen storage and usage. In this method, hydrogen can be added and stored to methane as an additive. Therefore, at the present study, the effects of step, added hydrogen to methane as an additive fuel and some physical properties such as thermal conductivity of the wall of combustor (K_w), convective (h_{out}) and radiative (e) heat transfer coefficient of outer surface of combustor on temperature distribution, combustion progress and flame location in a micro-tube combustor are investigated numerically.

Governing equations and numerical scheme

The physical geometry of the simulated micro-tube is shown in Figure 1. As it is shown, Methane-air mixture as a main reactant is entered into the micro tube.

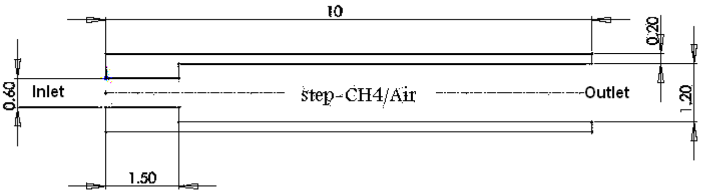

Figure 1. Dimension of a backward facing-step micro tube (in mm)

A skeletal mechanism accompanied by 25 reversible reactions and 15 species [18, 19] (without N compositions) has been applied for modeling of Methane-air combustion process. The equivalence ratio is set in 0.9 (fuel lean mixture of methane-air) [20- 23]. Pre-mixed reactants temperature, wall thermal conductivity and emissivity coefficient, outer wall convection heat transfer coefficient are varied from 300 to 400 K, 3 to 160 W/m.K, 0.1 to 0.3 [23] and 5 to 25 W/m^2.K, respectively. Meanwhile, heat energy transfers from micro-tube outer wall to environment by radiative and convective methods. All reference thermal boundary conditions at the wall/environment interface are gathered in Table 1.

Table 1. Reference conditions.

Model	2D-Axisymmetry-Detail chemistry
Velocity or Mass Flow (V_{in} & $M_{dot,\ in}$)	2.8 m/s – 8.88e-7 kg/s
Thermal conductivity(Wall) (K_w)	20 W/m.K
External heat transfer coefficient (h_{out})	5 W/m^2.K
Emissivity coefficient (e)	0.2
Mass fraction of added hydrogen	0.005

Regarding Table 1, ambient temperature, reference emissivity coefficient and outer wall convective heat transfer coefficient are 300 K, 0.2 and 5 W/m^2.K, respectively. The lateral interactions between micro-combustor wall and environment at inlet and outlet are adiabatic.

The governing equations of an axisymmetric, laminar steady state multi-species reactive flow are as follows:

Continuity

$$\frac{\partial(\rho u)}{\partial x}+\frac{1}{r}\frac{\partial(\rho v r)}{\partial r}=0 \tag{1}$$

Axial momentum

$$\frac{\partial(\rho u u)}{\partial x}+\frac{1}{r}\frac{\partial(\rho u v r)}{\partial r}=-\frac{\partial p}{\partial x}+\frac{\partial}{\partial x}\left(\frac{4}{3}\mu\frac{\partial u}{\partial x}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\mu\frac{\partial u}{\partial r}\right)-\frac{\partial}{\partial x}\left(\frac{2\mu}{3r}\frac{\partial(vr)}{\partial r}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\mu\frac{\partial v}{\partial x}\right) \tag{2}$$

Radial momentum

$$\frac{\partial(\rho uv)}{\partial x}+\frac{1}{r}\frac{\partial(\rho vvr)}{\partial r}=-\frac{\partial p}{\partial r}+\frac{\partial}{\partial x}\left(\mu\frac{\partial u}{\partial r}\right)-\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{2r\mu}{3}\frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial x}\left(\mu\frac{\partial v}{\partial x}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{4r\mu}{3}\frac{\partial v}{\partial r}\right)-\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{2}{3}\mu v\right) \quad (3)$$

Energy equation

$$\frac{\partial}{\partial x}(\rho uh)+\frac{1}{r}\frac{\partial}{\partial r}(\rho vhr)=\frac{\partial}{\partial x}\left(k_f\frac{\partial T}{\partial x}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(k_f r\frac{\partial T}{\partial r}\right)+\dot{q} \quad (4)$$

Species conservation

$$\frac{\partial(\rho uY_i)}{\partial x}+\frac{1}{r}\frac{\partial(\rho vrY_i)}{\partial r}=\frac{\partial}{\partial x}\left[D_{i,m}\frac{\partial(\rho Y_i)}{\partial x}\right]+\frac{1}{r}\frac{\partial}{\partial r}\left[D_{i,m}r\frac{\partial(\rho Y_i)}{\partial r}\right]+\omega_i \quad (5)$$

The energy equation through the solid wall of micro-tube

$$\frac{\partial}{\partial x}\left(k_s\frac{\partial T_s}{\partial x}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(k_s r\frac{\partial T_s}{\partial r}\right)=h_{out}(T_s-T_\infty)+\sigma e\left(T_s^4-T_\infty^4\right) \quad (6)$$

The diffusivity of radicals in normal direction into the wall is ignored. The overall boundary conditions, at the micro-tube inlet, inner section of the micro-tube wall and outer part of the micro tube wall are respectively as follows:

$Where\ (x\ and\ r=0)\rightarrow T=300K, u=2.8\ {}^{m}/_{sec}, v=0, \frac{\partial u}{\partial r}=0, \frac{\partial v}{\partial r}=0, \frac{\partial T}{\partial r}=0, \frac{\partial Y_i}{\partial r}=0$

$Where\ (r=0.3\ mm)\rightarrow\ u=0, v=0$

$Where\ (\ r=0.8)\rightarrow q_{wall}=q_{exit}$

$Where\ (x=0\ ,\ 0.3<r<0.8\ mm\ and\ x=\ 10\ mm\ , 0.6<r<0.8)\rightarrow\ \frac{\partial T}{\partial x}=0$

The governing equations are solved by a finite-volume numerical scheme based on Patankar Simpler algorithm that is developed in a collocated mesh by Rahman et al. [24]. The convergence criterion for all equations was set on 10^{-6} [25]. As it is shown in Figure 2, for achieving high accurate and efficient results, a grid independency study has been carried out using several different grids. A grid with 5120 cells (3620 cells in flow field zone and 1500 cells in solid zone) has been used. More grids show no significant difference among the results which had been extracted from the other grids[2, 5, 26] .

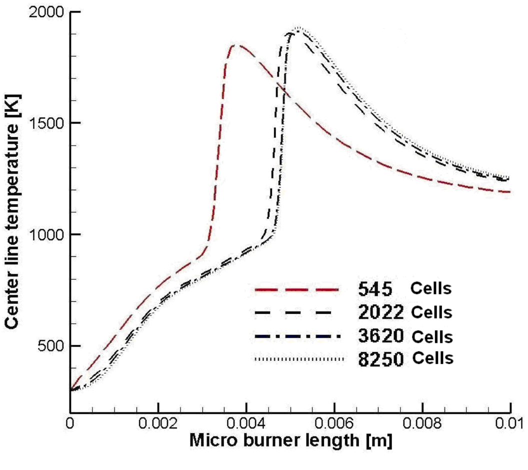

Figure 2. The Mesh study procedure.

Here, it should be noticed that the flame location in this study is attributed to a location with the highest temperature in the combustion field [27].The validity of applied code has been verified by the results of [28]. As it is shown in Figure 3, Maximum deviation of the results of applied code as compared to the experimental results of [28] is about 3.5%. This precision is adequately higher than the precision of similar works [23, 27 and 29] which have applied Smooke et al. [19] or other skeletal mechanisms for methane-air or hydrogen-air combustion modeling.

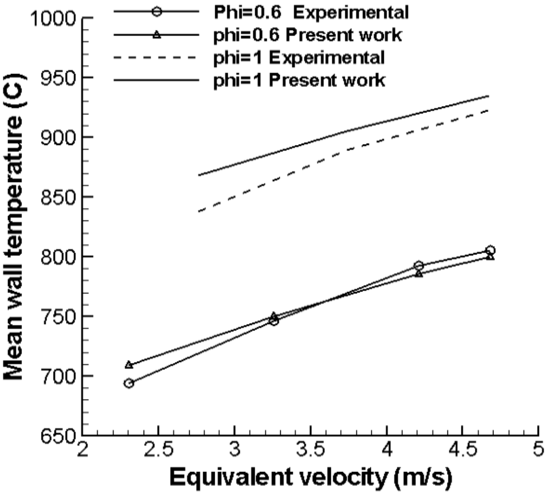

Figure 3.the validation of applied code performance by the results of Ref. [28].

Results and discussion

The effect of wall thermal conductivity

The wall thermal conductivity of a micro tube plays a competitive role in flame stabilization process [27]. On one hand, the increasing thermal conductivity of micro-tube wall facilitate heat recirculation and heat transfer [3, 21] from post-flame to pre-flame zones, properly, so that the low thermal conductivity of micro-tube wall leads combustion process to blow out due to less heat recirculation [4, 9, 25]. On the other hand, high wall thermal conductivity increases heat losses to outer ambient and in this way, can threaten combustion stability and presence of the flame in a micro-tube combustor [4, 9, 11]. The high surface to volume ratio in a micro-tube combustor exacerbates this situation and makes flame very susceptible to quenching. Thereby, keeping satisfying balance between heat loss and heat recirculation procedures seems to be the best solution [7, 30]. In this regard, several modeling have been conducted. The extracted results are gathered in Figure 4. As it can be seen, varying wall thermal conductivities cannot seriously affect the flame location and temperature distribution along the micro tube axis in hydrogen addition method as much as simple micro-stepped tube. This behavior can be attributed to the influences of added hydrogen and step on combustion phenomena, and also weak heat transfer characteristic of the outer wall of the micro-tube. Adding hydrogen to incoming reactive mixture of methane-air can move occurrence of the maximum Arrhenius rate and also distribution of some reactions such as $H+O_2 \rightarrow OH+O$, $O+H_2 \rightarrow OH+H$, $OH+H_2 \rightarrow H_2O+H$, $H+O_2+M \rightarrow HO_2+M$, $CH_3O+M \rightarrow CH_2O+H+M$ and $HO_2+H \rightarrow OH+OH$ towards the inlet port of the micro stepped tube. In fact, adding hydrogen to methane-air main reactive mixture can decrease initial ignition energy which is essential for combustion initiation. Also, adding hydrogen to methane-air mixture method can intensify the generation of “H” radical as an active and prominent radical in combustion field and this way strengthen the flame stability within the micro-tube combustor [31]. These coincident effects cause the combustion process in the micro-stepped tube to be resistant to increasing the wall thermal conductivity. Although, the wall thermal conductivity has not crucial role in the variation of temperature distribution and flame location along the micro-tube axis in hydrogen addition case, its effect on temperature distribution along the micro-tube wall in this case is meaningful. Moreover, although adding hydrogen can pull flame location into the inlet port, due to closeness of flame location to the entrance section of the micro tube and consequently limited preheating interval of the incoming fresh mixture, preheating process can’t be performed as good as simple micro-stepped tube by the micro-tube wall. Therefore the maximum temperature along the micro-tube axis in this method will be decreased trivially as compared to the simple micro-stepped tube. Furthermore, due to this fact that delineating the chemical species just on the micro-tube axis and wall can’t give good clues to hand for precise analysis and judgment about the effects of hydrogen addition on combustion process inside the micro tube, thereby, for better understanding of the distribution of chemical species through the micro-combustor, the average value of mole fractions have been presented in the following. Definition of mass-weighted average parameter is as below:

$$\frac{\int \rho\phi|\upsilon.dA|}{\int \rho|\upsilon.dA|} = \frac{\sum_{i=1}^{n} \phi_i \rho_i |\upsilon_i \cdot A_i|}{\sum_{i=1}^{n} \rho_i |\upsilon_i \cdot A_i|} \tag{7}$$

The mass-weighted averaging is an appropriate method [32] for representing the results of chemical species distribution in the micro-combustor.

As it is shown in Figure 5, adding hydrogen to the reactive mixture of methane-air can increase the average value of mole fraction of some chemical species such as H, OH, H_2O, HO_2, H_2O_2, CO_2, CH_2O, HCO in the flow field of the micro-combustor as compared with the simple micro stepped tube. Most of these species play the role of initiator for combustion commencement in the micro-combustor. Regarding Figure 5, although variation of the micro-tube wall thermal conductivity affects the average value of mole fraction of some species in the micro-tube for both simple step and hydrogen addition with step methods, its effect on simple step method is more prevalent and obvious. According to Figure 5, increasing the wall thermal conductivity coefficient increases the average value of some radicals such as CH_3O, HCO, OH, CH_3, CH_2O, HO_2 and H_2O_2 in simple micro stepped tube. This phenomenon is due to this fact that under such boundary conditions of the outer wall of micro-tube which heat transfer to ambient is not so extensive, increment of the micro-tube wall thermal conductivity will lead to better condition for heat transfer from post flame zone to preheating zone in a simple micro-stepped tube. This phenomenon moves flame location towards the inlet port of micro tube and this way increases the average mole fraction of some mentioned important radicals which are as markers for improvement of combustion characteristics inside the micro-tube. In contrast with simple micro-stepped tube behavior, micro-stepped tube with added hydrogen is almost insensitive to variation of the wall thermal conductivity of micro-tube as compared with the simple micro-stepped tube. Moreover, though some species in added hydrogen method don’t change obviously by the wall thermal conductivity variation, still increasing the wall thermal conductivity can decrease the average mole fractions of some species such as H, OH and O and also increase the average mole fraction of CH_3, coincidently. On the whole, according to faint heat transfer condition of the outer surface of the micro combustor, increasing the wall thermal conductivity has an increasing effect on conversion rate of methane and hydrogen in both simple stepped tube and stepped tube with added hydrogen methods.

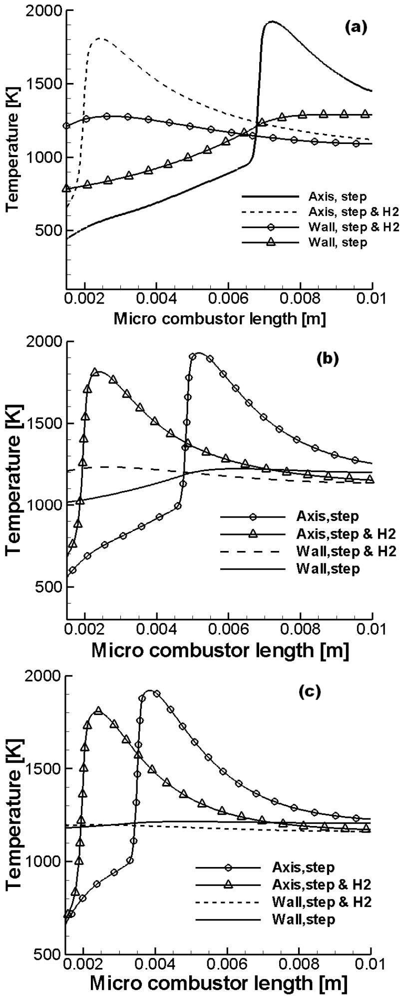

Figure 4. Distribution of temperature along the axis and the wall length of micro-combustor (u_{in} = 2.8 m/sec): (a) K_w = 7.5 W/m.K; (b) K_w = 20 W/m.K; (c) K_w = 90 W/m.K.

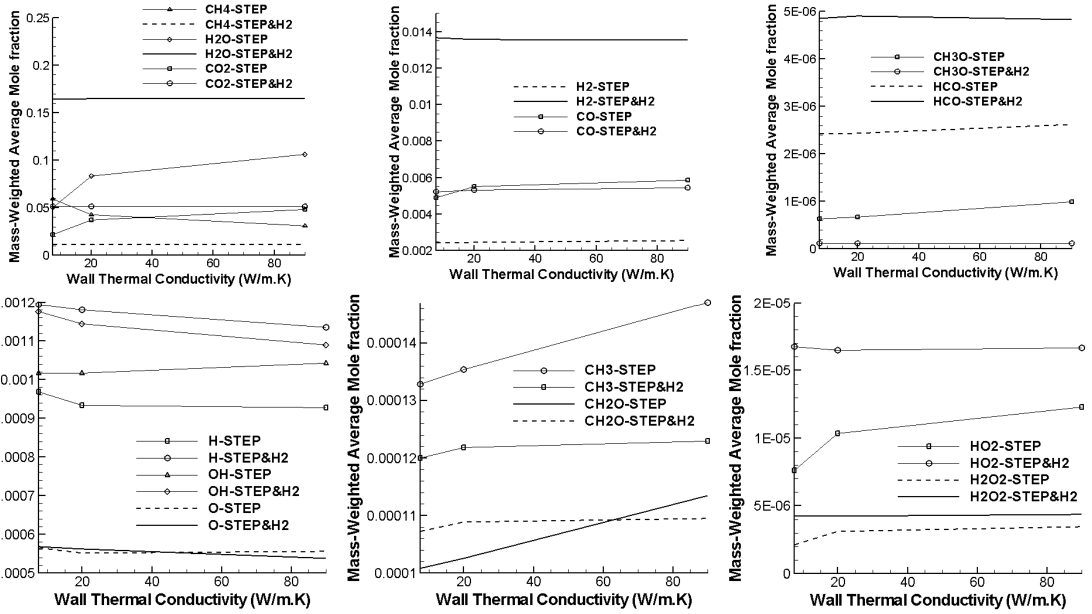

Figure 5. The variation of average value of species versus wall thermal conductivity in a micro- combustor.

The effect of convective heat transfer coefficient

The effects of convective heat transfer coefficient of outer surface on combustion phenomena inside a micro-tube combustor as a most important parameter of heat loss procedure to outer environment is discussed. The initial values of this modeling are set up based on the reference boundary condition values at Table 1. The gained results are graphed in Figure 6 which will be considered in following. From Figures 6 a,b, it is implied that the increment of convective heat transfer coefficient affects temperature distribution and flame location [4, 8, 10]. In this figure, the distribution of temperature and OH active radical mole fraction along the micro-stepped tube length are presented as initiator of combustion phenomena and flame location [11, 31], respectively. As it is seen, although the effect of convective heat transfer coefficient variation on the flame location in the added hydrogen method is negligible, on the contrary, its effect on the temperature level and distribution along the micro-stepped tube axis and wall is dominant so that it can decrease them obviously.

Moreover, distribution of OH radical species along the micro-stepped tube wall and axis are depicted in Figures 6 c,d, respectively. The graphs show that the distribution of OH species along the wall is influenced by convective heat transfer coefficient more than micro-stepped tube axis. This effect sounds to be reasonable due to this fact that heat loss effects on the inner wall of the micro-stepped tube are more dominant. Therefore, the radical and thermal quenching process always commences by the micro-tube walls [9].

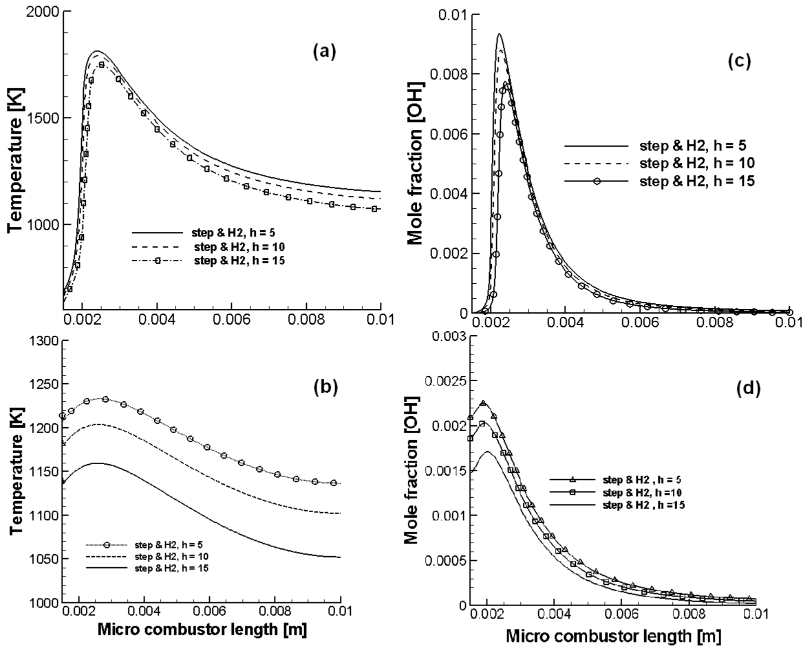

Figure 6. Distribution of temperature and OH mole fraction along the axis and the wall of micro-stepped tube length for hydrogen addition modifier method and for various outer wall convective heat transfer coefficients, (a,c) axis; (b,d) wall (h_{out}: 5, 10, and 15 $W/m^2.K$).

The effect of external emissivity coefficient

According to this fact that micro-TPVs are one of the main applications of micro-tube combustors, therefore, investigation into the effects of radiative heat transfer from the micro-tube wall to environment and also its influence on combustion field seems to be essential [21]. Generally, the heat transfer from the micro-tube wall to environment as a loss causes that active radicals such as OH and O to be diminished near the micro-tube wall and then this extinction of active radicals leads to combustion instability and finally flame extinguishment [9].

The profile of OH radical and temperature distribution at various emissivity coefficients along the micro-stepped tube axis for added hydrogen method is depicted in Figure 7 a,c. All the results have been solved under reference boundary conditions at Table 1. As it is seen, increasing emissivity coefficient causes decreasing trend in OH radical mole fraction due to increasing heat transfer from the micro-stepped tube wall to environment as radiation loss. More increment of emissivity coefficient leads to flame extinction. Increasing emissivity coefficient for the added hydrogen method just decreases the temperature level and OH radical mole fraction so that its influence on flame location is so trivial and negligible (approaching extinction).

Also, temperature distribution and OH radical mole fraction along the micro-stepped tube wall are depicted in Figures 7 b,d. From Figure 7 about the effects of emissivity on combustion process in the micro-tube, it can be inferred that increasing emissivity coefficient decreases temperature level on both of the micro-stepped tube wall and centerline. This phenomenon is attributed to higher radiative heat transfer rate due to strong dependence between temperature and radiative heat transfer. According to radiative heat transfer equation, radiative heat transfer increases by fourth power of temperature [33]. On the whole, due to high surface to volume ratio in micro-tubes, the combustion process within micro-tubes is always threatened by quenching of active radicals [9] such as O and OH. Therefore, the conditions in the micro-tube should be chosen properly in that to assure flame stability in blow out and extinction situations somehow [7, 30].

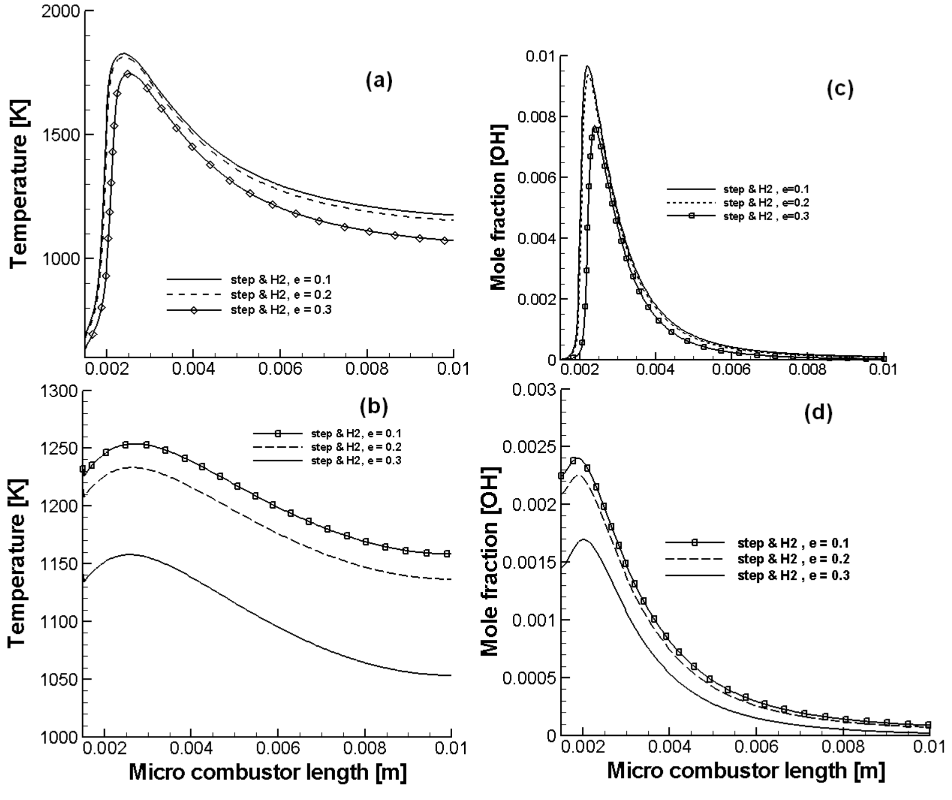

Figure 7. Distribution of temperature and OH mole fraction along the axis and the wall of micro-stepped tube for added hydrogen modifier method and for various the micro-tube wall emissivity coefficients, (a,c) axis; (b,d) wall (e: 0.1, 0.2, and 0.3), (h_{out}: 5 W/m^2.K).

Conclusion

The modification ability of added hydrogen method for improving the methane-air pre-mixed combustion in a micro-tube combustor has been investigated numerically. The effects of adding hydrogen to methane as an additive and some physical properties such as thermal conductivity of wall of combustor (K_w), convective (h_{out}) and radiative (e) heat transfer coefficient of outer surface of combustor on temperature distribution and combustion progress in a micro-stepped tube are calculated using a 2D laminar pre-mixed numerical code. The Numerical results show that applying added hydrogen to methane in a micro-stepped tube combustor has significant and impressive effect on improving and stabilizing of the flame in a micro combustors and can play pivotal role in modification of combustion phenomena in a micro combustor. As compared to single back ward facing step method and also according to the wall thermal conductivity (K_w), hydrogen addition method can improve flame location inside the micro-tube 35% to 55% and increase uniformity of temperature distribution on the micro-tube wall. Also, it is found that adding hydrogen to CH_4 can assure the flame presence in some certain conditions in comparison to the simple backward facing step method. Moreover, the results indicate that the outer wall conductivity and emissivity have destructive effect on the flame properties inside the micro-combustor, so that they can decrease active radicals' concentration in combustion zone, impressively. However, on the whole, the hydrogen addition method demonstrates more efficient performance than simple micro-stepped tube so that it can increase the resistance of the flame against the variation of the outer wall heat transfer conditions and this way increases the combustion efficiency in the micro tube.

Nomenclature

A	Area (m^2)
D	mass diffusivity, m^2/s
e	Emissivity coefficient
h	Specific enthalpy, J/kg
h_{out}	Outer wall convective heat transfer coefficient ($W/m^2.K$)
$k_{f\ or\ s}$	Thermal conductivity of fluid or solid (W/m.K)
p	Pressure (pa, p_{atm} = 101325 pa)
$\dot{q}$	Heat generation rate per unit of volume, W/m^3
r	Radial direction, (m)
T	Temperature, K
u	x-direction velocity, m/s
v	r-direction velocity, m/s
x	Axial direction, m
φ	Property

Y_i	mass fraction of i^{th} species
μ	Dynamic viscosity, $N.s/m^2$
ρ	Density, kg/m^3
σ	Stephan-Boltzmann coefficient
ω_i	species mass generation rate of i^{th} species per unit volume

Subscript

exit	Outer surface of the combustor
i	species i^{th}
i,m	species i in the mixture
in	Inlet
s	Solid
w	Wall
∞	ambient

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