A numerical study of methane-air premixed flame in a diverging micro-channel

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ABSTRACT
In the present paper, numerical study on the characterization of flame stabilization behaviour in a 2.0 mm wide diverging channel are carried out with premixed methane-air mixtures by solving the appropriate form of two-dimensional governing equations. The effects of combustor divergent angle, equivalence ratio and boundary conditions (wall and inlet) on the flame temperature are reported in this work. The simulation results show that the temperature of the flame was highest for a fuel-air mixture having stoichiometric ratio. The diverging portion of channel is preheated from the bottom side with a sintered metal burner to provide a positive temperature gradient along the direction of fluid flow which helps in stabilizing a flame in the channel. Further, it was noted that flame is stable for velocity limits between 0.2 m/s and 1.9 m/s for a range of mixture equivalence ratios. There was no significant change in flame temperature irrespective of divergent angle. The boundary conditions such as wall temperature affected the stabilization of flame.

1. Introduction:
In the present Era, the most powerful tool for the industrial development is Energy. For various equipment like vehicle, robots, computers, laptops, communication devices, space technology systems, we need a powerful energy system, which may be in the form of batteries. For developing such energy devices, we need to focus on some important factors like size, energy density, mass transfer coefficient, cost effectiveness of the system and time required to recharge the system. For this, we are searching possibilities in hydrocarbon fuels in place of advanced Li-ion concept based electrochemical batteries [1, 2]. So, now we are switching on micro-combustion field. A lot of work has been carried out in the field of micro-combustors which may be a better option for portable production of energy because we know that hydrocarbons have significantly larger energy density in comparison of traditional Li-batteries [7], Maruta et al. [8] did experimental work on the characteristics of flame propagation by using premixed methane-air mixture as a fuel in a 2.0 mm diameter straight quartz channel with a wall temperature gradient. He found stability of flame on higher and lower velocities and pulsating flames on intermediate velocities. Similarly, Hua et al. [9] work on micro tube combustor combustion with different diameters for different wall thermal conductivities and heat transfer coefficient. Some other researcher have done a lot of work in the field of flame stabilization behaviour in micro can combustor [13] radial channel combustor [14], micro gas turbine engines [3, 10] & micro thermo photovoltaic system [11, 12] and some other important concepts of micro combustors [15-22]. Pan et al. [12] have done research work on the effect of wall thickness to combustor diameter ratio, hydrogen to oxygen mixing ratio on micro combustion. Chao et al. [15] found in his experiment that a preheat of tube/channel is required to stabilize the flame for example for 2.0 mm diameter quartz tube 1173K preheat temperature required to stabilize methane –air flame. In addition of this, an experimental work on methane –air combustion in a diverging micro channel done by B. Khandelwal, S. Kumar [23]. In this paper, the numerical simulation of wall temp done in respect of experiment done by B. Khandelwal, S. Kumar [23]. We are also trying to find out the effect of diverging angle and equivalence ratio on the stabilization of flame by using methane-air as a fuel.

2. Mathematical formulation:
Fig. 1 shows cross-sectional view of a typical two-dimension- al sintered metal heating burner with a dotted curve near the outlet of the channel. In this channel, methane and air burning takes place. In Fig. 1, x-axis denotes the longitudinal direction (from starting point of diverging section) and y-axis denotes the transverse direction. Premixed methane-air mixture flows along the positive x direction. The origin is fixed at centre line of the combustor inlet. X and Y co-ordinates show axial and radial variations respectively in micro combustor. The flow is considered steady and axisymmetric which renders the problem 2D symmetric. By certain design and computational assumptions the swirl component of velocity is taken as zero. The computations are performed only in half of the domain for the sake of economic usage of computational time. The following assumptions are also invoked to further simplify the problem:

1) There is No work done by pressure and viscous forces
(2) No gas radiation occurs.
(3) Dufour's effect neglected.

With these assumptions, the equations of continuity, momentum, species, and energy in the gas phase (for the divergent micro-combustor) can be written as follows:

Continuity Equation:
\[
\frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho rv)}{\partial r} = 0
\]

Momentum Equation:
\[
\left( \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho rv)}{\partial r} \right) = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left( \frac{\mu}{3r} \right)
\]

Radial Momentum Equation:
\[
\left( \frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho rv)}{\partial r} \right) = -\frac{\partial p}{\partial r} + \frac{\partial}{\partial x} \left( \frac{\mu}{r} \right)
\]

Energy Equation:
\[
\left( \frac{\partial (\rho u^2)}{\partial x} + \frac{\partial (\rho r v^2)}{\partial r} \right) = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) - \frac{1}{r} \frac{\partial}{\partial r} \left( r \rho \sum_{i=1}^{N} Y_i h_i V_i \right)
\]

Species Conservation Equation:
\[
\frac{\partial (\rho Y_i)}{\partial x} + \frac{\partial (\rho r v Y_i)}{\partial r} = 0
\]

Boundary Conditions:

The boundary conditions are given as follows:

Inlet:
At inlet (x = 0): \( T_u = 300K, u_o = 0.2 \) to 1.8 m/s.

\( \phi = 0.8 \) to 1.8. \( Y_{CH4} \) & \( Y_{O2} \) can be derived for an equivalence ratio.

Centre line:
At symmetry plane, both diffusive as well as convective fluxes are considered zero, i.e. \( r = 0, \frac{\partial u}{\partial r} = 0, \frac{\partial T}{\partial r} = 0, \frac{\partial Y_i}{\partial r} = 0, \)

\( v = 0 \).

Gas-solid interface:
No-slip boundary conditions apply at walls, and diffusive flux normal to the interface are considered zero. The heat flux at the interface is computed by making an energy balance between convective heat flux with the convective heat flux at the wall.

At \( r = r_0 \), \( u = 0, \frac{\partial Y_i}{\partial r} = 0 \).

Heat losses from the wall exposed to the surroundings are taken as:
Where, heat transfer coefficient \( h_{wall} \) and the wall emissivity \( \varepsilon \) are assumed as 50 W/m²K for free convective environment and 0.2 for polished surface with slightly oxidized surface.

Fig. 1. Schematic of the 2-D computational domain of diverging micro-channel.

3. Results & Discussion:

Reference case:
Every result needs a reference to validate itself. For this purpose, we are going to validate results from reference case experimental work [paper]. There are three wall temperature profiles shown in the figures 2a, 2b, and 2c in comparison with the experimental wall temperature profiles. Fig. 3 shows the inside wall temperature profile along the longitudinal direction of the micro channel from the reference point ‘0’ for cold flow conditions at different velocities. These are used for proper measurement of initial wall temperature profile. The premixed methane-air mixture is subjected to these wall temperature profile conditions. In the curve we are seeing that the wall temperature increases in the divergent section. This is because of the heat provided by sintered metal burner to the combustor. The measured temperature varies along the centreline of the micro channel from an average of 400 K (+_50 K) to 600 K (+_100 K) with an increase in the flow.

Fig. b
Fig. 2 compares the wall temperature of the channel along the direction of flow with different flow rate conditions for experimental and simulation work.

Fig. 2a, 2b, 2c shows the results for wall temperature for cold flow conditions. Simulation results are very close to the experimental results. Variation in the wall temperature is +/- 100K which is allowed between experimental and simulation results.

Effect of equivalence ratio on flame temperature:
Fig. 3a, b, c shows the result for the effect of the equivalence ratio on the flame temperature. Temperature limits for $\phi=0.8$ to $\phi=1.2$ is 300 K to 2900 K. It can be easily understood that for leaner as well as richer mixture of premixed ch4-air we get a maximum temperature limit 2600 K but this reaches maximum 2800 K for stoichiometric value, $\phi=1$. It can be concluded that in diverging micro-channel, it is possible to stabilize the flame at lower temperature limits for lean as well as rich mixture. As in experimental work we got completely stable flame for $\phi=1.1$ & $u=0.23$ [paper]. It shows that we get stable flame for rich equivalence ratio and lower velocity for lower temperature of flames.

Effect of diverging angle on flame temperature:
Diverging angle also has significant effect on the flame temperature and flame stability. As previous work reveals us about flame stability in a cylindrical tube / channel. In comparison of cylindrical channel, diverging micro-channel gives us stable flame result on lower maximum temperature of flame. Fig. 4a, b, c shows results for diverging angle $\alpha=5^\circ$, $10^\circ$, $15^\circ$, for these angle maximum flame temperatures are 2255 K, 2245 K, 2225 K respectively. These results show that as we shift from lower diverging angle to the higher degree of angle, we get lower maximum temperature of flame with flame stability. This helps us to choose the angle for the proper burning of the ch4-air mixture.

Effect of equivalence ratio ($\phi$) on centreline flame temperature:
For stoichiometric ratio $\phi=1$, we see that flame has its maximum temperature. Fig. 5 shows the effect of equivalence ratio on centreline temperature of the flame.
For inlet values: axial velocity \((u) = 1\) m/s, diverging angle of micro combustor \((\alpha) = 15^\circ\), we see that centreline temperature of flame for equivalence ratio 1 is maximum in comparison of centreline temperature for equivalence ratio 0.8, 1.2. Here the value of maximum centreline temperature of flame for \(\phi = 0.8\) & 1.2 is nearly same. But it has maximum value in case of \(\phi = 1.0\). It means combustion zone in case of leaner & richer mixture is large to accommodate the effect of temperature. This also indicates towards the fact that for the lower centreline temperature of flame we can reduce the size of the combustor. One more advantage is that we can get stable flame even on lower temperature with proper combustion of fuel. This may lead the economy of combustion and limitation of material for combustion.

**Effect of diverging angle \((\alpha)\) on centreline flame temperature:**

Fig. 6 shows the effect of diverging angle \((\alpha)\) on centreline temperature of the flame. For inlet values: axial velocity \((u) = 1\) m/s, equivalence ratio \((\phi) = 0.8\), we see that centreline temperature of flame has maximum value ~1500 K for diverging angle \((\alpha) = 5^\circ\) & \(15^\circ\). For diverging angle \((\alpha) = 10^\circ\), centreline temperature of flame is ~1250 K. Here we see that centreline flame temperature is less in case of \(\alpha = 10^\circ\) in comparison of other angle but from fig. 6 maximum temperature occurs for \(\alpha = 5^\circ\) & \(10^\circ\) which is 2255 K & 2245K respectively. Here maximum temperature plays vital role in case of designing of combustor and in selection of combustor material. So from these point of view we prefer the diverging angle \((\alpha) = 15^\circ\), as it is economical for combustion point of view.

**Effect of equivalence ratio \((\phi)\) on flame velocity about centreline:**

Flame velocity plays a crucial role in combustion. If flame velocity is too high then there will be certainly unburned in the flue gases and if velocity is too low then combustion may occurs before it reaches to combustion zone. This may cause instability of the flame. Fig. 7 shows the effect of equivalence ratio \((\phi)\) on flame velocity profile about centreline. For the inlet axial velocity \((u) = 1\) m/s, combustor divergence angle \((\alpha) = 15^\circ\), we see that axial velocity for \(\phi = 1\) is highest and for \(\phi = 0.8\) it is minimum. For these values deviation of maximum axial velocity occurs from 2.8 to 3 m/s, this is very small difference. So we equivalence ratio does not have much influence on axial velocity about centreline. So we choose \(\phi\) for which flame is stable.

**Effect of diverging angle \((\alpha)\) on flame velocity about centreline:**

For the proper combustion of fuel and stability of flame, velocity is a dominant factor and this factor can get affected by divergence angle of combustor i.e. combustor geometry. Fig. 8 shows the effect of diverging angle \((\alpha)\) on flame velocity about centreline. For the inlet axial velocity \((u) = 1\) m/s, equivalence ratio \((\phi) = 0.8\), we see that maximum axial velocity for \(\alpha = 5^\circ, 10^\circ, 15^\circ\) are 3.4 m/s, 3.8 m/s, 2.75 m/s approximately. Here axial velocity has remarkable difference with respect to divergence angle \((\alpha)\). Here one more important point is noticed that axial velocities for \(\alpha = 5^\circ, 10^\circ\), are steep in nature and increases till end of the combustor, so there may be chance of fuel getting out from combustor. This fuel may burn outside the burner which will result in unbalanced flame with improper combustion. So it is satisfactory to choose diverging angle for which flame found stable as well as combustion is proper.

**Conclusion:**

In this work, premixed combustion of ch4-air in a divergent channel investigated. Effect of various factor like wall temperature, diverging angle, equivalence ratio discussed in this paper work. From the above discussion following conclusion can be summarized:

1. Wall temperature is a key factor which helps to stabilize the flame in the combustor. This also ensures the uniform heating of the fuel entered into the combustor and uniform burning which results in lower emission rate and finally healthy environment condition.
2. Equivalence ratio can be taken as a dominant and controlling factor which directly relates to the flame stabi-
lization and its temperature. As in above discussion we see that maximum temperature of flame occurs for unit equivalence ratio or stoichiometric ratio in this case. So for the economy point of view we can switch over other optimal option to get well stabilized flame with less emission. Here rich equivalence ratio provides us stable flame with comparatively lower maximum temperature of combustion.

3. In case of diverging micro channel combustor, diverging angle also become a good factor for the designing of combustor as well as controlling factor for flame temperature about centreline in combustion zone. Here we find out a conclusion that as we increasing the diverging angles from 5° to 15°, maximum temperature of the combustion flame reduces which helps to stabilize the flame. In this work, for 15° angle, flame temperature about centreline (1500 K) is maximum in comparison of others but it does not have such importance as maximum temperature (2225 K) of flame is far greater than it.

4. Similarly, the effect of divergence angle of combustor can be concluded. Here the divergence angle play important role as for lower value of diverging angle of combustor velocity is high than that of velocity for higher value of diverging angle. So it reveals about the fact that diverging angle must be 15° for the given case.