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Research paper



Flame Structures of Burner Stabilized Laminar Premixed Flames

***Vinod Kumar Yadav[1], Prabhat Ranjan[2],Vijay Yadav[3] , Omprakash Yadav[4]**

[1] G. L. Bajaj Institute of Technology & Management, INDIA
[2]Indian Institute of Technology, Delhi, New Delhi 110062, INDIA
**Corresponding author E-mail: yadavvinod2004@gmail.com*

Abstract

In this paper, numerical analysis of flames stabilized over flat-flame burners at 298 K and 1 bar are studied using ANSYS Fluent® software. The temperature, velocity and kinetic rate of reaction of methane (CH_4)-air mixtures were analyzed by varying the unburnt mixture velocity. The conditions similar to experiments, performed on heat flux method, were created for numerical analysis and the measured results were compared with experimental results. Three-dimensional steady state simulations with one-step chemistry were conducted to predict the curvature effects and flame structure. One-dimensional laminar burning velocity data was also predicted using ANSYS Chemkin -Pro® software with GRI Mech. 3.0 reaction mechanism. The experimental and numerical values of laminar burning velocity were 0.358 m/s and 0.361 m/s respectively at 1 bar and 298 K. Through numerical simulation, the thickness of the reaction zone at predicted laminar burning velocity was 0.84 mm and the peak reactions appeared around 0.88 mm above the burner top surface. The maximum predicted temperature was 2250 K which in turn is slightly higher due to the fact that the simulations were conducted using one step chemistry.

Keywords: *Laminar burning velocity, flat flame, 3D simulation.*

1. Introduction

Laminar burning velocity (LBV) of any mixture is the relative velocity with which unburnt gas moves to the flame front normally. LBV is an important property of any combustible mixture [1-2] which helps in determining the overall reaction rate, kinetic schemes and it also governs combustion phenomena. LBV is measured by various techniques like Bunsen burner, counter-flow, spherical flame and heat flux method. Out of these heat flux method, which in turn is a variant of flat-flame burner, developed by de Goey and co-workers [3], produces flat stretch less flame in which the flame gets stabilized by heating the burner plate using hot water inside the jackets around burner periphery. After measurements the temperature profile is plotted and laminar burning velocity is determined using interpolation. Bosschaart and de Goey [4] presented the constructional details and proposed modifications in the burner design in order to isolate the hot part from the cold one. Maaren et al. [5] designed a unique variant of flat-flame burner to measure the flame temperature and burning velocity of laminar premixed flames under adiabatic condition. They measured the temperature profile of the burner plate and calculated the heat loss. They found the temperature profile to be uniform over the burner plate, which signifies the development of flame under adiabatic (zero heat loss) condition. DeGoey et al. [6] numerically studied the small scale structure of CH_4-air flames stabilized above a flat-flame burner and discussed about the pore size, porosities and mixture velocities in order to generate undistorted flat flames. They concluded that the flames stabilized over the flat flame burners adopted by Maaren et al. [5] with d/p (d= hole diameter in mm, p= pitch in mm) of 0.4/0.5and 0.5/0.7wereused with hydrocarbon/air mixtures upto burning velocity of 40 cm/s. They also observed curvature effects on the flame when H_2/CH_4 mixtures having burning velocities in the range 200 cm/s were experimented over the flat-flame burners. Wider variation between experimental and numerical results were observed with high burning velocities due to increased flame-surface of curved flames. Maaren et al. [7],also reported the nature of flame distortions and concluded that these are invisible due to their small scale. The maximum burning velocity that can be measured with flat flame burner was limited to 60-65 cm/s [8], however, no experimental results have been found to justify this maximum value. Vladimir et al. [8]reported that the experiments conducted on flat flame burners possesses an uncertainty in LBV in the range of 0.5-1 cm/s. Konnov et al. [9] conducted 2D simulations of flow through heat flux burner for low pressures and predicted gradual increase in burning velocity with decreasing pressure. Goswami et al. [10] conducted 2D axis-symmetric simulations at elevated pressures on stoichiometric methane-air flat flames using the heat flux method. They numerically modeled 3 burner designs at high pressures(around 7 bar) using one-step chemistry. They reported that by choosing small hole diameter and large porosity, the increase in flame surface area may be reduced appreciably. They measured the laminar burning velocity up to 70 cm/s on the fabricated plates and suggested that in order to extend the burning velocity beyond 70 cm/s, the plenum chamber and burner plate re-design may be done. Most of the simulations reported so far on flat flame burner were conducted with 2D model. The primary focus of this work is to conduct 3D simulations on flat flame burner in order to broaden the understanding of flame structure more precisely. The flatness of the CH_4-air flames under stoichiometry using a burner plate d = 0.5 mm and pitch = 0.7 mm, similar to that used in the experi-

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ments, was verified through numerical simulations. Kishore et al. [11] used the same burner for cellularity study.

2. Numerical Modeling

In the present work, 3D computations were conducted using CFD software ANSYS Fluent®[18], which solves the governing equations for species, mass, momentum and energy. Steady state simulations with one-step kinetic mechanism were conducted to predict the flame structure. For conducting the simulations, pressure based numerical solver, with parallel processing (8 processors) is used. The pressure-velocity coupling is solved using SIMPLE algorithm. The segregated solver with double-precision was adopted with implicit method to ensure the solutions of discretized algebraic equations. Control volume approachis used by the software to convert the complex governing equations into simplified algebraic equations. The second-order upwind scheme was opted for solving the governing equations. The 3D simulations for the burner plate width = 0.5 mm and p = 0.7 mm was started with an initial velocity of 0.35 m/s, CH_4mass fraction of 0.055 and O_2 mass fraction of 0.22. Table 1 shows some of the burner plate models used by combustion groups including Goswami et al. [10] for their2D simulations.

Table 1: Flat flame burner plate specifications

Plate No.	Specifications			Reference
	Diameter (mm)	Pitch (mm)	Plate thickness (mm)	
1	0.5	0.70	2	[3-5]
2	0.5	0.60	2	[10]
3	0.3	0.36	1	[10]
4	0.3	0.40	1	[10]

It was observed during the experiments that the flame generally appears 0.5 to 1 mm above burner plate hence a domain length of 8 mm was set. The initial guess of velocity was set at 0.35 m/s due to the fact that during experimentation with stoichiometric methane-air mixtures, the burning velocity was measured as 0.36±0.01m/s.

3. Validation

The experiments were conducted at 298±1 K and 1 bar on a flat flame burner with d/p of 0.5/0.7 and the obtained results were compared with ANSYS Chemkin-Pro® [12] using full GRI Mech. 3.0 reaction mechanism [13]and experimental results [2, 14]. The detailed specifications of the experimental setup and its photograph can be referred from the research articles published by the corresponding author in references [2, 17]. Fig. 1 compares the present experimental results with the results available in literature. The measured results are in close match with the results of Hermanns et al. [14] and also with the computations of ANSYS Chemkin-Pro software. The prime focus of the present simulations is to understand the flame structure of a 3D flame, hence stoichiometric-methane air mixture was selected, for which published results are available in abundance.

4. Results and Discussions

To start the combustion, patching with a temperature of 1900 K was done above the burner plate. The patching was repeated till the mixture got ignited. After running 25000-30000 iterations, the solution got converged. However, the results obtained were dramatic. There was a trace of methane left after the reaction zone till the end of the domain, showing incomplete combustion even at stoichiometric conditions. The input variables were again analyzed and it was observed that there is some discrepancy with specific heat polynomial coefficients of Fluent's data base [18]. The Fluent theory manual suggests that the value of polynomial coefficient for high temperature calculations may be adopted from Rose & Cooper [15]. The simulations were restarted with Rose & Cooper polynomial coefficients in the temperature range of 300K to 3000 K. The solution converged with nice trends for methane mass fraction over a vertical line along the axial distance. However, when the same values were used for lean and rich methane-air mixtures, the trace of methane was noticed. Then, the polynomial coefficients provided by NASA [16] were adopted and nice trends under all equivalence ratios were obtained. Table 2 presents the NASA polynomial coefficients adopted for CH_4-air mixtures under different temperature range.

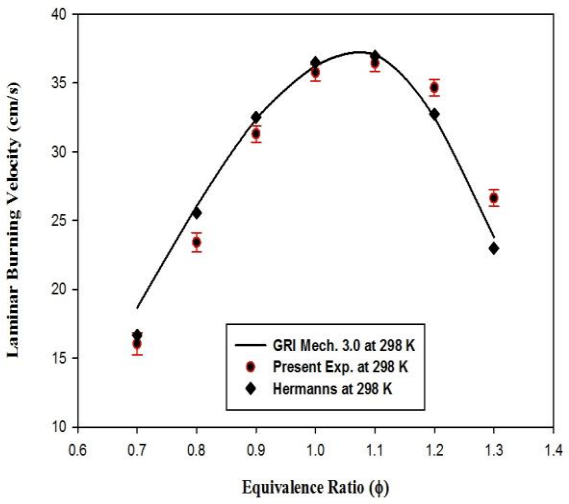


Fig. 1: Validation experiments for CH_4-air mixture at 298 K, 1 bar and under stoichiometric condition. (Experimental data of Hermanns et al. [14] under similar conditions)

Table 2: NASA [16] specific heat coefficient values used for 3D simulations

Coefficient	Temperature range	
	298K-1000K	1000K -3000K
a_1	5.15E+00	1.64E+00
a_2	-1.37E-02	1.01E-02
a_3	4.92E-05	-3.37E-06
a_4	-4.85E-08	5.35E-10
a_5	1.67E-11	-3.16E-14

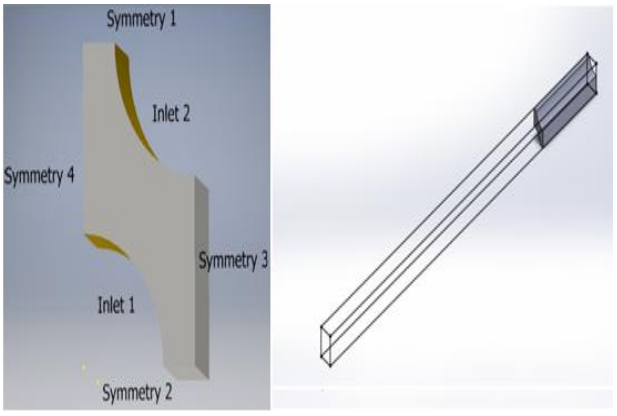


Fig. 2: 3d model of burner plate

The schematic of computational domain for three-dimensional heat flux burner stabilized premixed flame and chosen boundary conditions are shown in Fig. 2. For saving the computational time and cost, the model was optimized to its minimum possible extent by defining symmetry on all four sides. Fig.3 shows the symmetrical planes as a rectangle ACEG chosen for modeling the geometry. Inlet 1 and inlet 2 represents the two holes from where the

unburnt mixture enters inside the burner plate. The burner plate-1of 2 mm thickness, d = 0.5 mm and p = 0.7 mm was selected for present study. The burner plate with identical specifications was used by our group in the experimental work [2, 17]. At the end of the domain pressure outlet boundary condition was specified. The burner plate was maintained at 358 K by circulating hot water around burner's periphery. This is because during experimentation, the burner plate is maintained around 358 ± 1 K to minimize the heat loss from the flame to the plate[2].Additionally, the flame region (about 3 mm above the burner top) was refined to resolve large gradients that are typically present near the burner plate. However, a coarser grid was adopted in regions away from the flame to save the computational memory and time.

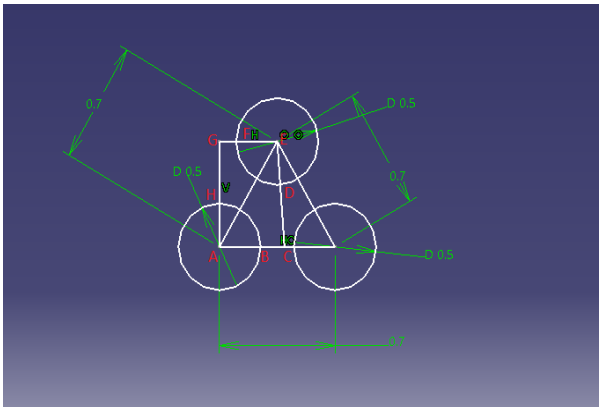


Fig. 3: Burner plate geometry

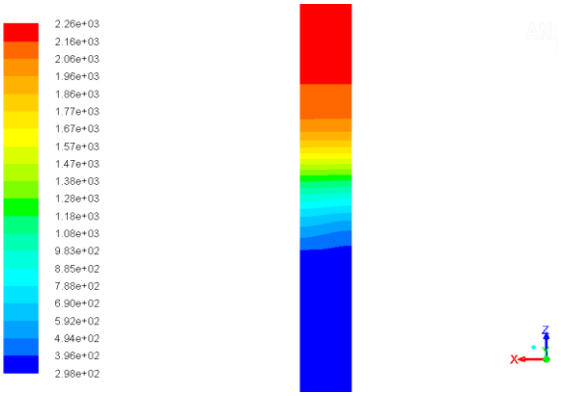


Fig. 4: Contours of static temperature

Fig. 4 shows the contours of the static temperature plotted along a cutting plane above the burner plate, and is at the centre of the burner plate. The minimum and maximum computed temperatures were 298 K and 2250 K respectively. The temperature is over predicted due the use of one-step chemistry, as discussed byde Goey et al. [6] in their computational work.

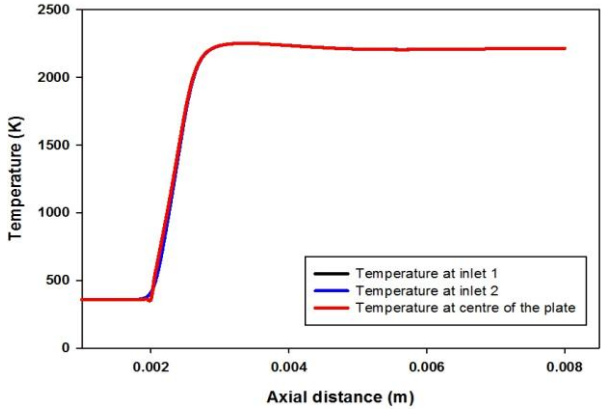


Fig. 5: Static temperature profile over the burner plate at hole centre and at the plate centre

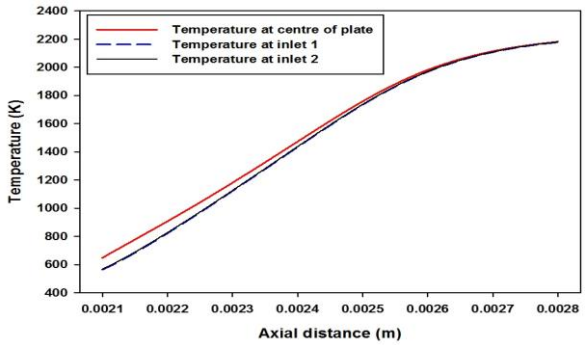


Fig. 6: Temperature inside the reaction zone at 0.1 mm to 0.8 mm above burner plate

The temperature inside the reaction zone is plotted in Fig.5 along flame's downstream (z-axis) direction. To estimate the temperature along the axial direction, three vertical lines were drawn above the burner plate. Two of them were at the centre of the two inlets (inlet 1 and inlet 2) and the third line is drawn at the centre of the burner plate (solid part). The temperature profiles at both holes were identical. However, there is a negligibly small variation in the temperature profile plotted from the centre compared to inlet 1 and 2. To magnify the differences in temperature profile between the holes and plate centre, three more vertical lines are drawn specifically inside the reaction zone where maximum temperature gradient and maximum reaction rate is expected. These lines were drawn at 0.1 mm above the burner plate and are of 0.7 mm length as shown in Fig.6. Inside the reaction zone, the recorded temperatures along the two inlets were repetitive. The temperature along the vertical line drawn at the centre of the burner plate was initially higher but becomes comparable with those calculated at two inlets, while moving towards the outlet side (at a height of 0.6 mm to 0.9 mm above the burner plate).The maximum rate of reaction was observed at an axial distance of 0.6-0.9 mm from the burner plate top. This can be verified from the calculated results of kinetic rate of reaction plotted in Fig.7 and 8, which clearly shows that the reactions are on their peak at a height of about 0.6-0.9 mm above burner plate in the gas velocity range 0.34 - 0.38 m/s.

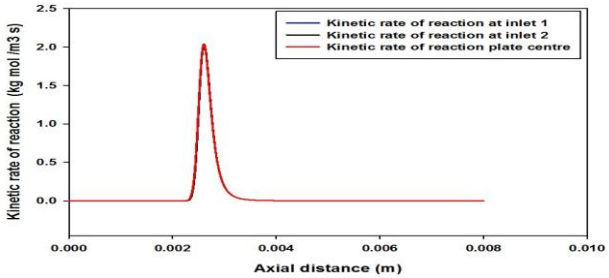


Fig. 7: Calculated kinetic rate of reaction for CH_4-air mixture (stoichiometric) at inlet 1, inlet 2 and centre of burner plate. At a pressure of 1 bar and temperature of 298 K.

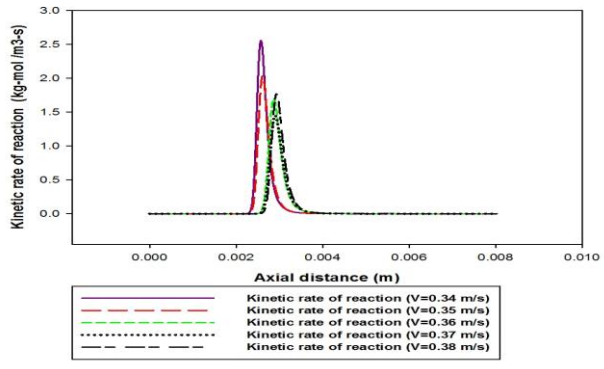


Fig. 8: Calculated kinetic rate of reaction for CH_4-air mixture (stoichiometric). At a pressure of 1 bar and temperature of 298 K.

Fig. 8 shows the kinetic rate of reaction for unburnt mixture velocities in the range of 0.34 to 0.38 m/s. At an unburnt mixture velocity of 0.34 m/s, the reaction rate is more compared to other velocities, due to the nearness of the flame from the burner top plate. At velocities 0.35 to 0.36m/s, the reaction rates are comparable, indicating that the flame might have become flatter compared with to other velocities. With further increase in velocity, the reaction rates decreases. This is due to the fact that the flame has lifted sufficiently above the burner plate, causing more diffusion of atmospheric air from the surrounding that cools the flame.

It was observed that the temperature variation in a plane at a height of 0.7 to 0.9 mm above the burner plate is about 13 K to 2K respectively (Table 3), which justifies that there is a small temperature gradient inside reaction zone. Meanwhile, towards downstream side, the temperature gradient is limited to 2 K, supporting that the flame has become flat at about 0.7 to 0.9 mm above the burner plate.

From Fig. 9, it can be seen that the temperature contours are comparable for unburnt mixture velocities of 0.35 m/s and 0.36 m/s. With further increase in unburnt mixture velocity, the maximum temperature falls and the flame moves away from the burner plate. This further supports that the burning velocity lies within 0.35 m/s to 0.36 m/s. The estimated burning velocity is comparable with the values predicted with the help of experiments and ANSYS Chemkin-Pro® simulations.

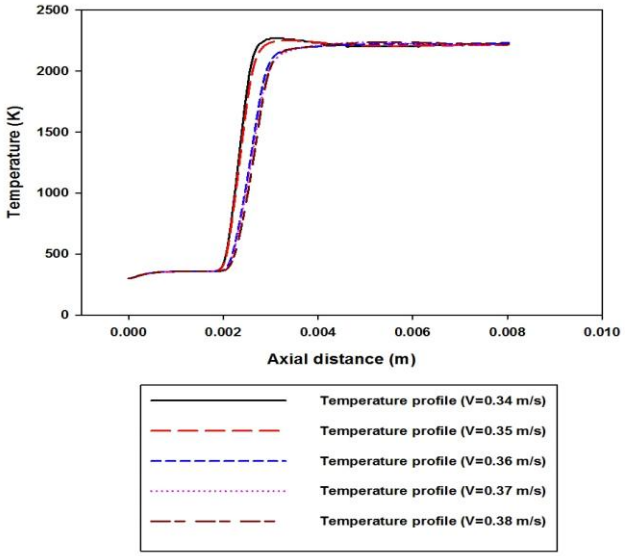


Fig. 9: Static temperature profile over the burner plate at holes and at plate centre for different velocities

Table 3: Calculated temperature at a plane drawn at different heights in axial direction above the burner plate.

Plane height above burner plate (mm)	Temperature range (K)	
	Min	Max
0.1	562	655
0.2	822	915
0.3	1122	1187
0.4	1435	1477
0.5	1733	1759
0.6	1968	1981
0.7	2107	2113
0.8	2179	2182
0.9	2214	2216
1.0	2232	2232
1.1	2242	2244
1.2	2247	2250

Table 3 shows the temperature over a plane at various heights above burner top. The temperature over a plane at 0.6 mm above the burner top is in the range 1968 to 1981 K and the kinetic rate of reaction is 2.0107 to 2.033 kg mol /m^3.Fig. 10 shows the calculated results of major species mole fraction that were created or consumedin reaction zone during methane-air combustion simulated using single-step chemistry. The predictions of maximum temperature is higher than the adiabatic flame temperature of 2226 K [1]. This is due to the use of single step chemistry mechanism as reported in many research literatures [6] and also in Fluent's theory manual. The Fig. 9 also indicated that the pre-flame reactions start immediately after passing through the burner holes and becomes rapid with increase in temperature at the location where the reactions rates are higher. From Fig. 4 and Fig.6, it can be inferred that the results are repetitive at inlet 1, inlet 2 and burner centre plate in the reaction and flame zone. Hence, to calculate the production and consumption of major species, the species profiles are plottedfor stoichiometric CH_4-airmixture along a vertical line drawn from the centre of the burner plate (Fig. 10).

4.1 Net Heat Transfer Rates

The net heat transfer rates form the burner surfaces are computed to predict the burning velocity of the mixture under adiabatic condition. The net heat transfer rate results along with unburnt mixture velocity is shown in Table 4 and plotted in Fig.11.

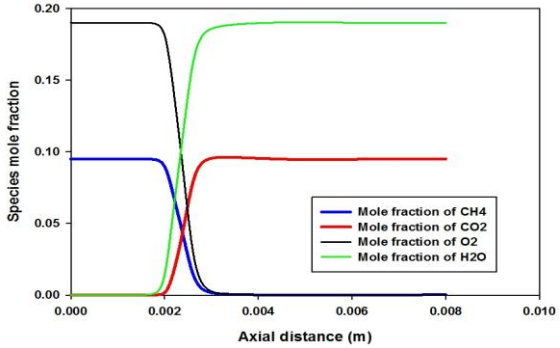


Fig. 10: Calculated species mole fraction for stoichiometric methane-air mixture

By interpolation, it was observed that the laminar burning velocity under no heat loss condition (adiabatic) for stoichiometric CH_4-air mixture comes out to be 0.361 m/s (Fig. 11). During experiments, the measured laminar burning velocity (adiabatic) was 0.358 ± 0.01 m/s. The 3d results are in good agreement with the measured results. This supports that the results of one step chemistry can be considered as a good estimate of the actual laminar burning velocity of fuel-air mixtures.

Table 4: Unburnt mixture velocity and net heat transfer rate

Unburnt mixture velocity (m/s)	Net heat transfer rate (W)
0.34	-0.00768274
0.35	-0.006303922
0.36	0.003382284
0.37	0.004196154
0.38	0.005009878

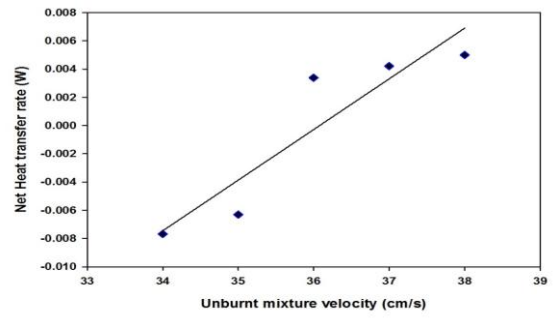


Fig. 11: Computed unburnt gas velocity and net heat transfer rate

Fig. 12 shows the velocity vector above the burner plate for an unburnt mixture velocity of 0.36 m/s. It also supports that there is no directional non-uniformity along z direction. The peak reaction rate for unburnt mixture velocity of 0.36 m/s appeared at 0.88 mm above the burner top and the reaction zone thickness was observed as 0.84mm.

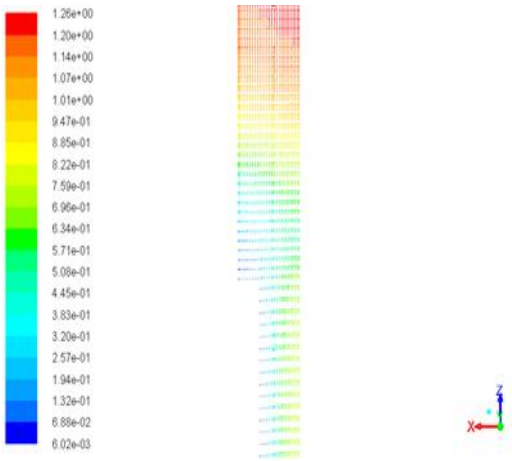


Fig. 12: Velocity vector for unburnt mixture velocity of 0.36 m/s

5. Conclusion

3d simulations over the flat flame burner based on heat flux technique used in experiments for predicting the burning velocity of various premixed gaseous fuel mixtures is conducted usingANSYSFluent®software [18]. For creating good quality mesh, the domain is optimized to its minimum possible extent by creating symmetry at all the four sides of the geometry. Pressure-based numerical solver is used for computations. To reduce the calculation time, parallel processing is adopted with one-step methane-air combustion chemistry. The following conclusions are made:

1. Maximum kinetic rate of reaction occurs at a height of 0.6-0.8 mm above the burner plate for gas velocities in the range 0.34-0.38 m/s.
2. Maximum temperature of stoichiometric methane-air mixture is about 2250 K. However, the adiabatic flame temperature reported in literature [1] is 2226 K. Literature [10] supports that the prediction of temperature with one-step chemistry is higher.
3.Temperature variation in a plane at a height of 0.7 to 0.9 mm above the burner plate is about 13 K and 2K respectively. This indicates the generation of wrinkle-free flat flame over the burner plate similar to experiments.

These results may be useful in understanding the flame structure when the flat flame burner is operated around its upper limit of burning velocity measurements (0.60-0.65 m/s), and provides an insight of the net heat interactions under the conditions which are difficult to visualize during practical experimentation.

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