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Simulation Studies Of Premixed N-Pentane/Air Liquid Micro Combustion

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ABSTRACT

With latest improvements in MEMS, combustion based *Micro-Power generation* devices are seen as alternatives for conventional batteries because of the high energy densities of Hydrogen and other hydrocarbon fuels. An important feature of micro-power system is to utilize the combustion of fuel or propellant in the micro-burner to produce the gas with high temperature and high pressure to drive turbines or other power units, which convert chemical into energy directly or indirectly other forms of energy, for example heat or power. We have concentrated on the usage of Micro combustion as a substitute for conventional batteries .In our study, a *Micro Combustor* of *1mm x 10mm* is taken for Numerical Study. Combustion characteristics of *N Pentane-Air mixture* in a planar micro-channel is studied numerically. We have performed the liquid fuel combustion of n-Pentane and air to study the effects of liquid fuel combustion in a micro channel. The effect of axial velocity inlet, on exhaust gas temperature and Hydrogen Peroxide addition on exhaust gas concentration was analyzed respectively. We also investigated numerically the combustion characteristics under different conditions such as by varying the *DPM, Number of Fuel Streams, and Spray Angle* and so on. For this numerical analysis, an experimental model is considered as reference, and the geometry and the boundary conditions are taken from it for the purpose of simulation. In this study, n-Pentane is introduced as liquid droplets at the centerline and the liquid combustion is simulated numerically.

Keywords - Liquid fuel Microcombustion, n-Pentane/air with Hydrogen Peroxide, Premixed flame, Flame Temperature, k-epsilon model

NOMENCLATURE :

d-- Inner diameter (m)
h-- Enthalpy (J/kg)
hconv--convective heat loss coefficient (non-insulated wall) (W/ (m2K))
hi-- enthalpy of the *i*th species (J/kg)
H-- Spacing between the parallel plates (m)
k-- Thermal conductivity of gas (W/ (mK))
kB--Boltzmann constant (1.380662×10!23 J/K)
L-- Combustor length (m)
P --Pressure (Pa)
q-- Volumetric heat generation rate (W/m3)
Ru-- universal gas constant (8314.41 J/ (kg mol K))
t-- **Wall thickness (m)**
T-- **Temperature (K)**
*T*0-- **ambient temperature (K)**
Tu-- **temperature of unburned mixture (K)**
Tw -- **wall temperature at the interface (K)**
Two -- **temperature of the non-insulated wall (K)**
u-- ***x* velocity (m/s)**
*u*0-- **incoming flow velocity (m/s)**
Ui--***x* velocity of the *i*th species (m/s)**
V—***y* velocity (m/s)**
Vi-- ***y* velocity of the *i*th species (m/s)**
x-- ***x*coordinate (m)**
y -- **Coordinate for 2D parallel plates (m)**
Yi --**mass fraction of the *i*th species (kg/kg)**

I. BACKGROUND

N Pentane is one of the hydrocarbons which can be used as a fuel. The hydrocarbons have high power- weight ratio compared to our conventional batteries. Methane, Ethane, Butane and Hexane are some of the other fuels. As the hydrogen content of a fuel increases, the calorific value as well as the energy provided by the fuel gradually increases. Also, considering if we are going to replace conventional batteries with Micro-combustion based power systems, we have to go for liquid fuel micro combustion because, it may be difficult to handle gases for long power cycles. Hence, we have chosen n-Pentane as the liquid fuel for our Micro combustion study.

Comparatively, Pentane has higher standard enthalpy of combustion and lower auto ignition temperature when, compared to Methane. Scope of our work is to study Hydrogen Peroxide effects on liquid fuel combustion of n-Pentane and air using Turbulence and Premixed conditions in Fluent 6.3

II. INTRODUCTION

Serious ecological imbalance and environmental degradation resulting from the burning of fossil fuels have increased the concern towards Combustion. Lean combustion is generally considered as one of the timely solutions for more stringent environmental regulations and global warming concerns. It is a fact that hydrocarbon fuels contain 100 times more energy per unit mass than lithium-ion batteries. Hence, micro-combustion based power systems can be implemented to replace conventional battery system which also, reduces overall system weight, increased operational life times and reduced unit cost[1]. It may find a large application on Portable electronic systems whose, majority of overall system weight consists of Batteries. Therefore, harnessing power from Micro combustion efficiently, is an ideal way to pave the way for miniaturization of a power source package. However, at small scales, heat and friction losses become more significant, thus devices based on existing macro scale designs such as internal combustion engines may be impractical[2]. Essentially, our study is aimed at achieving a stable combustion in simple geometries such as cylindrical tubes or rectangular channels. It was studied that, as the combustor length increases, the range of flow conditions for successful ignition becomes smaller[3]. Also, stable combustion can be obtained for mixtures with equivalence ratio outside conventional flammability limits with externally heated micro channels[4]. In case of micro flames, the diffusion rate becomes very fast, so that the finite chemical reaction rate starts to govern the phenomenon[5].

Pentane comparatively has the worse ignition properties and also has low burning velocity. These conditions cause the instability and low power output for the combustion process. Thus, these weaknesses become disadvantages for micro combustion which require the maximum utilization of energy source. In other way, a normal combustion of pentane should be improved to maximize the output power so that the demand can be filled. Thus, the study of hydrogen peroxide effects on pentane-air combustion is needed to overcome the shortcoming of n-pentane/air combustion, so that the combustion method can be improved to sustain the utilization of fuel source for the future energy requirement. Thus, in the experimentation and performance analysis of pentane combustion behaviour in the ambient condition, several parameters like equivalence ratio, axial velocity conditions, spray angle variations, fuel stream variations are needed to quantify the results.

III. MODELLING

Goemetry:

Figure 1 shows the two - dimensional view of the micro-channel (cylindrical tube and 2D parallel plates) in which steady-state combustion of a n-Pentane– air mixture takes place. Symbols d or H represents the diameter of the cylindrical tube or vertical distance between 2D parallel plates, respectively.

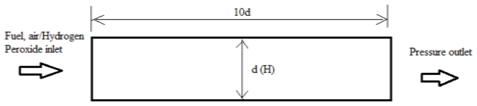


Fig. 1. Schematic of the computational domain with some boundary conditions (not to scale)

Governing equations:

As the characteristic length of the combustor chamber is sufficiently larger than the molecular mean-free path of gases flowing through the micro-combustor, the Knudsen number is very low and hence, fluids can be reasonably considered as continuum and the Navier-Stokes equations are still suitable in the present study. Since, Reynolds number is greater than 500 at the inlet, the turbulence model can be used to predict the combustion characteristics. It is expected that in a micro-combustor, the mixing of various kinds of species is enhanced due to the small space. Therefore, the realizable k-e turbulence model is adopted here. The governing equations for the gaseous mixture are shown below:

2.1 Continuity Equation:

$$\partial/\partial x(\rho v x) + \partial/\partial y(\rho v y) = 0 \qquad \text{-- (1)}$$

2.2 Momentum Equation:

2.2.1 X – Direction:

$$\partial/\partial x(vxvx)/\partial x + \partial/\partial y(vxvy)/\partial y = -\partial p/\partial x + \partial/\partial x(\tau xx) + \partial/\partial y(\tau xy) \qquad \text{--- (2)}$$

2.2.2 Y – Direction:

$$\partial/\partial x(vyvx)/\partial x + \partial/\partial y(vyvy)/\partial y = -\partial p/\partial y + \partial/\partial x(\tau xy) + \partial/\partial y(\tau yy) \qquad \text{--- (3)}$$

2.3 Energy:

$$\partial/\partial x(\rho vxh) + \partial/\partial y(\rho vyh) = \partial/\partial x^2(kf\partial T) + \partial/\partial y^2(\rho vxh) + \sum_{i=1}^{\infty}(\partial(\mathrm{hi}\rho\mathrm{Di,m}\,\partial\mathrm{Yi}\,\partial\mathrm{X})/\partial\mathrm{xi} + \partial(\mathrm{hi}\rho\mathrm{Di,m}\,\partial\mathrm{Yi}\,\partial\mathrm{X})/\partial\mathrm{y}) + \sum_{i=1}^{\infty}(\mathrm{hiRi}) \qquad \text{--- (4)}$$

2.4 Species: $\partial/\partial x(\rho Yivx) + \partial/\partial y(\rho Yivy) = -\partial/\partial x(\rho Di,\mathrm{m}(\partial Yi/\partial x)) + \partial/\partial y(\rho Di,m(\partial Yi/\partial y))$ --- (5)

IV. COMPUTATIONAL APPROACH

As n-Pentane has lower burning velocity, we have introduced Hydrogen Peroxide as a secondary oxidiser in addition to air which, acts as a primary oxidiser. It has been studied by Guan Bang Chen that, with the addition of Hydrogen Peroxide, the laminar burning velocity has been improved[6]. Thus, we have introduced Hydrogen Peroxide which improves the laminar burning velocity of n-Pentane. We have also studied the effects of flame temperature with the variation in the percentage /moles of air replaced by Hydrogen Peroxide.

Assumptions:

An assumption is made that the swirl velocity component is zero, meaning a symmetrical flow with respect to the centreline. Thus, the case is simplified to a 2D problem. No work is done by pressure and viscous forces. The simulation is done for steady state conditions.

The n-Pentane air reaction is:

$C_5H_{12} + 8\ O_2 \rightarrow 5\ CO_2 + 6\ H_2O$ + heat/ energy

The n-Pentane hydrogen peroxide reaction is:

$$CH_3(CH_2)_3CH_3 + 16\ H_2O_2 \longrightarrow 22\ H_2O + 5\ CO_2$$

(Source : Wolfram Alpha)

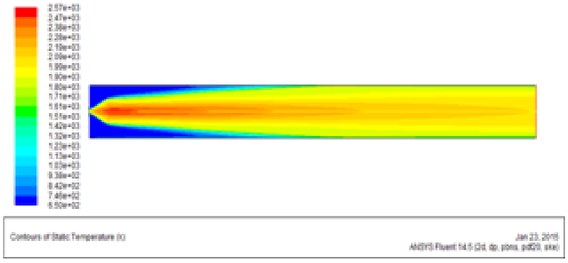
The mechanism for n-Pentane oxidation is employed in our study. Based on the above equations, 2-D simulations were performed. A second order upwind scheme is used to discretize the governing equations and SIMPLE algorithm is used. The equations are solved with Double Precision method using Pressure based equation solver. The convergence criteria for residual monitors are set to 1E-6 for the equations (1) to (5). The specific heat which, depends on Temperature is calculated as a piece-wise polynomial fit of temperature. At the inlet, the mixture enters with a uniform temperature of 303K. For the outlet, a pressure farfield condition has been set with a guage pressure of 0Pa. The wall conditions have been applied to the upper and lower surfaces of the rectangular plane. A temperature guess of about 1500K is set to ignite the mixture since, a low temperature would result in lack of ignition. The Injection is defined with the Particle type as Droplet and the number of streams is specified. The material is chosen as n-Pentane liquid whose diameter distribution is set to be linear. The diameter of 0.0001m is specified in the point properties. These are some of the physical and boundary conditions set for our study which, is common to all the cases.

V. RESULTS

It can be seen that, addition of active fuels (such as hydrogen) or adding strong oxidants to fuels is an alternative to enhance lean flame combustion without involving any design modification. Hydrogen peroxide (H_2O_2) is an environmentally friendly oxidant with strong oxidability whose, oxidizing power is lower to that of fluorine , which has the strongest electronegativity in the periodic table. Hydrogen peroxide under normal temperature is in liquid state, so that it is comparitively easy to store and handle in repeated case when, considering gas storage for MEMS which may diffuse and leak. Also, sufficient inlet pressure has to be applied for small scale applications. However, the small storage tanks have to be properly maintained and should allow for homogeneous decomposition of Hydrogen Peroxide if any, and should be able to resist high temperatures thus, should be placed away from heat source[7]. The decomposition reaction may be facilitated by heating or using catalyst and it is defined as:

H2O2 -> H2O + 0.5 02

TEMPERATURE CONTOUR (with H2O2)



TEMPERATURE CONTOUR (AIR)

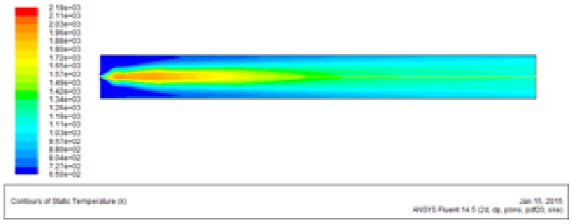
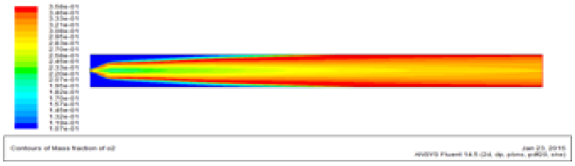


Fig. 2. Contours of Static Temperature in case of 50% replacement of air with Hydrogen Peroxide and normal combustion of n-Pentane and air

It can be observed that, the adiabatic flame temperature is 2570 K in case of n-Pentane and air with Hydrogen Peroxide where, 50% of air is replaced with Hydrogen Peroxide. In normal n-Pentane and air combustion, the adiabatic temperature reached is 2190K. It is comparable to standard adiabatic flame temperature of 2272K (@298.15K and 1atm pressure) [9].This shows that, there is an increase in 380K when half of air is replaced by Hydrogen Peroxide.

MASS FRACTION (O2) WITH H202



MASS FRACTION (O2) WITH AIR

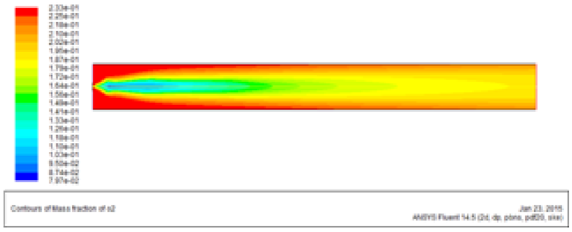
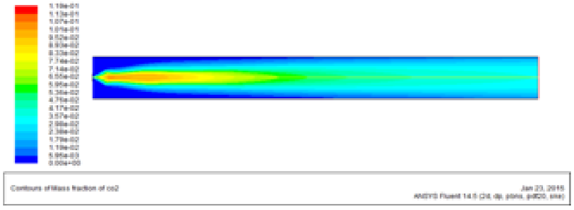


Fig. 3. Contours of Mass fraction of Oxygen at the conditions as stated in the previous figure

MASS FRACTION (C02) WITH AIR



MASS FRACTION (CO2) WITH H202

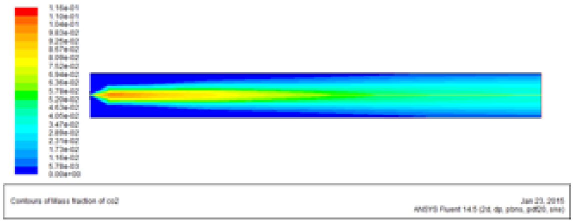


Fig. 4. Contours of Mass fraction of Carbon di-oxide at the conditions as stated in previous figure

There is a decrease in 2.58% of Carbon di-oxide in the case of n-Pentane and air with Hydrogen Peroxide.

It was also found that Heat lost/ Heat gained ratio was about 8.41E-2.

Grid Independence Test

Grid is the sub division of the domain into smaller sub domains - ***grid*** (or ***mesh***) of ***cells*** (or ***control volumes*** or elements) [8]. In general, the larger the number of cells, larger the accuracy. In a grid independence test, the computational cost is reduced without compromise in accuracy of solution. A mesh convergence test should mean computing the solution on successively finer grids.

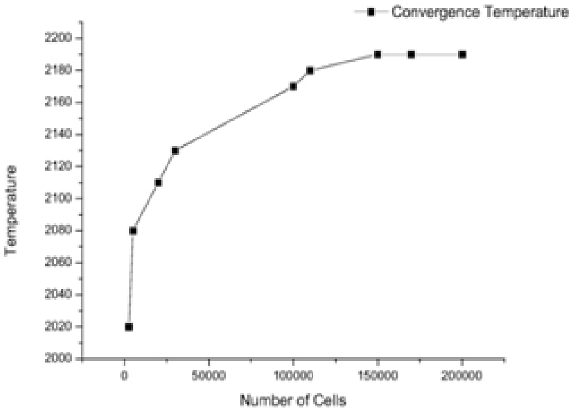


Fig. 5. Variation of Adiabatic Flame Temperature result with respect to variation in number of cells

Fuel Stream Variation

Following are the contours of Static Temperature obtained by varying the fuel streams:

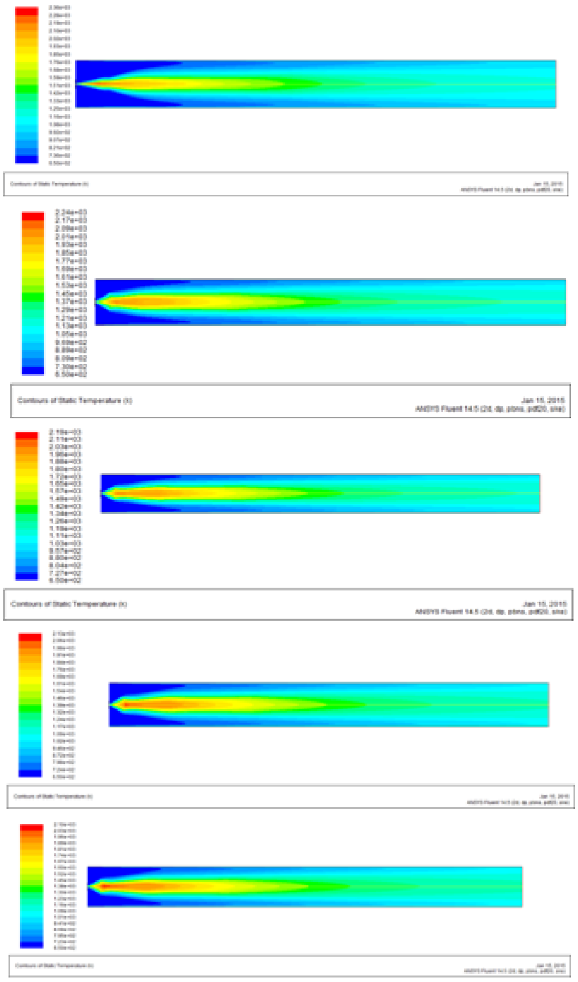


Fig. 6. Fuel stream variation

The continuous flow mixing is highly important for continuous combustion. The above plot indicates that as the number of streams increases, there is a high intermixing thereby leads to a complete and continuous combustion. As the number of streams is increased, more number of fuel droplets come into contact with the incoming air stream and therefore combustion takes place uniformly throughout the cross-section of the combustor. In case of minimal number of streams, whole of the mass flow rate is concentrated at some point of the combustor and hence the peak temperature gradually rises. Also, the thrust provided at the exit is not uniform which is not desirable.

When the number of fuel streams is increased, there is a reduction in the peak temperature. But there is uniform combustion in the combustor exit.

When the number of fuel streams is less, there is a high concentration of fuel at the axis of the inlet and thus, a lot of combustion reaction takes places at a confined region with minimal usage of oxidizer, thus the adiabatic flame temperature is increased in this case, where the combustion reaction and energy release is taking place in a reduced confined volume.

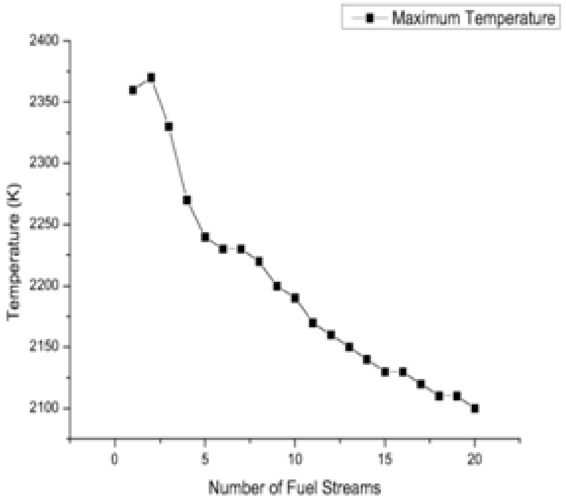


Fig. 7. Variation of adiabatic flame temperature with respect to fuel stream variation

From the Figure 7, it is clear that the Maximum Temperature decreases as the number of fuel streams is increased. From the figure, it is evident that the combustion is uniform throughout the combustor exit as the fuel streams are varied.

SPRAY ANGLE VARIATION

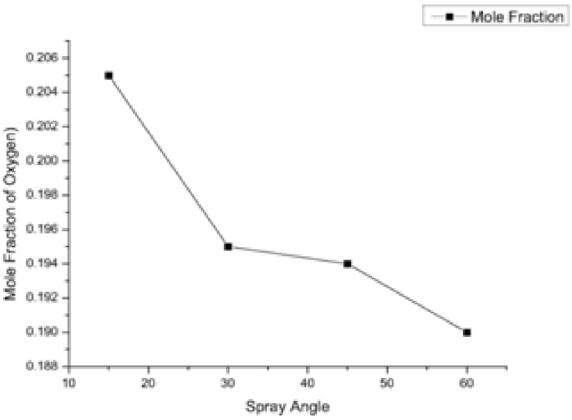


Fig. 8. Spray angle vs Mole fraction of Oxygen

In Spray Angle Variation, Simulations are done for a variety of spray angles such as 15°,30°,45° and 60°. All these are half cone angles. From the above figure 8, it is evident that the mole fraction of exhaust oxygen decreases as we increase the spray angle.

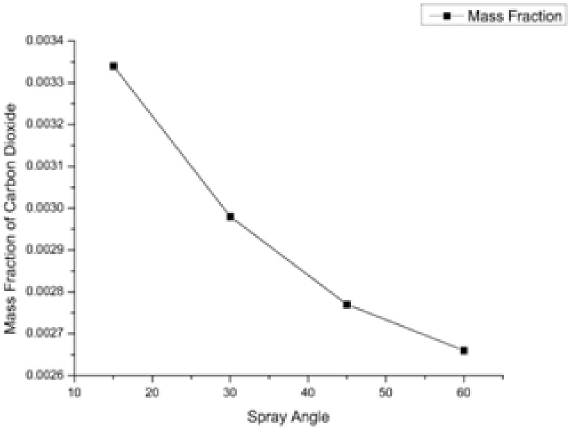


Fig. 9. Mass fraction of Carbon dioxide vs Spray Angle variation

From the Figure 9, it is evident that the Mass Fraction of Carbon-Di-Oxide decreases as the spray angle increases. Hence increase of spray angle favors the environment.

Mole Fraction Variation

The micro combustion was analyzed by varying the mole fraction of Hydrogen Peroxide used and the following results were obtained:

Mole fraction of H_2O_2	Adiabatic Flame temperature (K)	Mass fraction of CO_2 (xE-1)	Mass fraction of CO (xE-2)	Mass fraction of OH (xE-2)
0.5	2570	1.15	1.21	2.4
0.4	2530	1.16	1.10	1.92
0.3	2480	1.17	0.881	1.43
0.2	2410	1.18	0.758	0.967
0.1	2330	1.19	0.537	0.566

Table. 1. Variation of Adiabatic flame temperature and the mass fraction of different species with respect to Mole fraction variation of H_2O_2

It is seen that, as the mole fraction is increased, the Adiabatic flame temperature is increased thus, it is easier to stabilize a flame in micro channels using Hydrogen peroxide as a secondary oxidiser. Also, the mass fraction of OH concentration is improved, indicating a healthy combustion on increased addition of Hydrogen Peroxide. It can also be seen that, the mass fraction of Carbon Monoxide is increased when, compared with the mass fraction of Carbon di-oxide. This also indicates that, due to the addition of Hydrogen Peroxide there is an increase in concentration of the intermediate species.

It was also found from the simulation that, the particle residence time and particle vaporisation time were reduced from 0.0141s to 0.0132s and 0.0004s to 0.000236s respectively which indicates an enhancement of evaporation in the combustion process.

Axial velocity variation

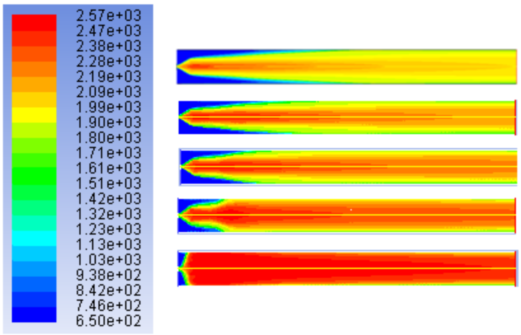


Fig . 10. Variation of flame vs Axial velocity

It is evident that as the axial velocity u0 increases, the combustion characteristics and flame are improved. For an velocity less than u0 = 0.4m/s, the air is stagnated at the inlet and the combustion region moves towards the wall. The axial velocity increases in the upstream of the flame front. In the region of high temperatures, the axial velocity is accelerated. It can be observed along the centerline for the first three cases which is uniform about the centerline. When the axial inlet velocity u0 is about 0.4m/s, the flame starts to move towards the wall and in the case of u0 = 0.2m/s, the flame is uniformly distributed throughout the chamber and has shifted from centerline towards the wall. However, various factors such as Heat recirculation in the walls of the combustion chamber, quenching distance, the convection effects and radial diffusion has to be studied to analyze the adiabatic flame temperature achieved in the combustion process.

Also, there was no greater variation in the particle residence time, particle vaporization time and particle temperature due to the variation in the axial velocity. This may be due to the scale or the order in which the axial velocity has been varied. Because, it is less when compared to the magnitudes of particle residence time and particle vaporization time which may be of the order of E-02 and E-04 respectively.

Thus, inlet velocity is crucial in determining the flame position apart from other boundary conditions specified.

VI. CONCLUSION

Since in the current trend, the demand for energy is greater than supply and the environmental factors, both contribute to the search for alternate fuels for efficient energy generation. Results indicate that the premixed flame with 10% air replaced by hydrogen peroxide has a higher adiabatic flame temperature comparatively. This is due to nitrogen dilution and heat release from thermal decomposition of hydrogen peroxide. The possibility of using n-Pentane in the liquid fuel micro combustion is studied. For the flame stabilization and increment in laminar burning velocity, Hydrogen Peroxide is used as an additional oxidiser. Thus, by increasing the number of fuel streams, setting optimal spray angle (around 50-60°), using lesser mole fraction of Hydrogen Peroxide to stabilize combustion, the liquid fuel micro combustion in micro channels can be greatly enhanced. Further studies can be carried out to reduce the Carbon Monoxide concentration at the exit by enhancing the turbulent mixing of the air and thereby, achieving complete combustion. Studies can also be carried out in the enhancement of evaporation of liquid fuel in the micro combustors.

Applications

This study is focused on micro scale applications where gaseous combustion is difficult and gives an insight of liquid fuel combustion in micro combustors.

VII. ACKNOWLEDGEMENT

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