Abstract— In this project Characteristics of micro-scale hydrogen diffusion flames produced by sub-millimetre diameter (d=0.2 & d=0.48 mm) are analysed & numerically simulated using ANSYS FLUENT v16. Simultaneous, temporally and spatially found out point measurements of temperature, major species concentrations (O2, N2, H2O, and H2), and absolute hydroxyl radical concentration (OH) are made in the micro flames for the first time. The calculated characteristic features and properties indicate that the buoyancy effect is minor while the flames are in the convection–diffusion controlled regime because of low Peclet number. Also, the effect of Peclet number on the flame shape is minor as the flame is in the convection–diffusion controlled regime. Comparisons of measured mean temperature, major species & OH mass fraction for d=0.2 & 0.48 mm with calculated radial profile are made at x=0.1, 1, 2 mm along the flame, where, ‘x’= Axial height of the flame from the burner surface.

Key words: Micro-Flames, Numerical Simulation, Convection-Diffusion Controlled Regime, Buoyancy Effect, Low-Peclet Number

I. INTRODUCTION

Recently, with increasing demands on micro-devices such as microsatellite and micro-aerial vehicle, needs for a micro-power source to activate these systems have significantly increased. These micro-systems require high-density power source to provide long periods of operation. Generally, the energy density of typical hydrocarbon fuels is about 100 times higher than that of batteries. Even regarding the heat losses in the process of extracting power from the fuel, a micro-scale combustion system has been considered as a viable alternative to batteries. To develop such combustion systems, an understanding of the physics of micro-flames must be made.

There have been some studies of micro flames experimentally, analytically, and numerically. Nakamura et al. [1] have performed experimental and theoretical studies on convection–diffusion controlled laminar micro flames to investigate the magnitude of diffusive-transport and its effect on the micro flame structure. They found that the buoyancy effect in the millimetre-size flames is negligible, while the axial diffusion is important in these flames. Yamashita et al. [2] conducted the extinction limit study of micro diffusion flames using microscopic shadowgraph and CH* emission imaging techniques. They reported that the quenching zone is located near the flame base, and the derived extinction curve can be described by Reynolds number times jet diameter. Mei et al. [6] used flame visualization and chemiluminescence measurement techniques along with analytical approaches to investigate the extinction process in micro-scale diffusion flames. They found that the measured quenching and blow-off limits are in agreement with the predicted values, and concluded that the behaviour of miniature diffusion flames can be adequately modelled by the laminar jet diffusion flame theory. In addition to the experimental and theoretical studies, Nakamura et al. [2-4] have performed a series of numerical simulations to investigate the burner size effects on micro flame structures using one-step and detailed reaction mechanisms. The predicted CH distribution and flame heights were in good agreement with experimental measurements.

Therefore, experimental measurements of temperature and reactive scalars are needed not only to gain a better insight into the physics but also to provide information for the input and validation of combustion models for CFD calculations. Furthermore, numerical simulations of the micro flames are performed and comparisons between the measured and predicted data are made to evaluate the capability of the CFD codes and to gain a better understanding of the characteristics of micro flames.

II. MODEL DESCRIPTION

A. Numerical Model & Boundary Conditions

A schematic of the numerical model used in the present study is shown in fig. 1.1.

The microscale hydrogen diffusion flames investigated here are stabilized on vertical straight stainless-steel tubes with inner diameters (d) of 0.2 and 0.48 mm, and the corresponding wall thicknesses 0.09 and 0.17 mm. Fuel is introduced through the tube into the quiescent atmospheric air with mass flowrates of 0.043 and 0.107 mg/s corresponding to the bulk velocity of 16.48 and 7.16 m/s for d = 0.2 and 0.48 mm, respectively. The Reynolds number, based on the exit conditions of fuel, is Re = 30 for both flames.

To numerically model micro scale hydrogen diffusion flames, the time-dependent ordinary sets of conservation equations (mass, momentum, energy, and species) are solved by making staggered grid system & based on Finite volume method. Axisymmetric 2-D plane (r–x) is considered as the computational domain because of the axi-symmetry of the jet. Co-axial Poiseuille flow of the pure hydrogen fuel is ejected upward into a quiescent atmospheric air (101 kPa, 300 K, 21%/79% of oxygen/nitrogen mixture). As seen in the figure, the burner is placed inside the computational domain, and therefore the property inside and also at the outside of the burner is calculated. This takes into account the back-diffusion of species into the tube.

Far-field boundary conditions are imposed to the open boundaries as shown in the figure. Non-slip, non-catalytic reaction & constant temperature (300K) conditions are applied on the burner surface. Normal gravity is considered as an external force. Burner specifications(inner/outer diameter, etc.) and volumetric flow
rate for the corresponding burner are set to meet the current experiments. Detailed transport and multi-step reaction mechanisms including nine species (H₂, O₂, N₂, H₂O, H, O, OH, HO₂, and H₂O₂) and 21 reversible reactions for hydrogen-air mixture are adopted for this study. Thermal properties for species are given by CHEMKIN database, while transport properties are determined by Smooke’s simplified transport model. Radiation heat loss from the H₂O is included based on the simplified optically thin model.

Fig. 1.1: Schematic of Numerical Model, Its Domain Boundary & A Micro Flame Established On a Jet Burner System

B. Governing Equations

The model calculations were made in time-dependent form with a stable convergence & they were continued until a steady-state solution was achieved. Governing equations are as follows (D/Dt denotes the substantial derivative in non-dimensional form:

1) Continuity (Mass conservation equation):
\[
\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{u} = 0
\]

2) Momentum Conservation Equation:
\[
\rho \frac{D\mathbf{u}}{Dt} = -\nabla \cdot \mathbf{T} + \rho \mathbf{g} + (\rho - \rho_w) \mathbf{g}
\]
where,
\[
\mathbf{T} = (\rho + 2/3 \mu \text{ div } \mathbf{u}) \mathbf{U} - \mu (\text{ div } \mathbf{u}) \mathbf{I}
\]

3) Energy Conservation Equation:
\[
\rho c_p \frac{DT}{Dt} - \mathbf{T} \cdot \nabla \mathbf{T} \cdot \mathbf{T} \cdot \mathbf{T}^T = q_{\omega}
\]

4) Species Conservation Equation:
\[
\frac{D\mathbf{Y}_i}{Dt} - \mathbf{T} \cdot \nabla (\rho \mathbf{D} \mathbf{Y}_i) = -\mathbf{v}_i \omega
\]

C. Adopted Numerical Scheme

Equations were solved using the finite-volume method in a staggered system. Central difference scheme is applied to the flux terms on the grid cell surface and the Euler implicit method is used for the time integration. In each time step, numerical iteration using the line-by-line successive over-relaxation (SOR) method is conducted. SIMPLE algorithm is employed for the pressure term in the Navier–Stokes equation. Total number of meshes is 81 for the radial and 141 for axial direction. Entire region of the calculation is about 40d and 60d for the radial and axial direction, respectively. Stretched meshes are applied in both the directions; a minimal grid size of d/10 is placed near the burner and an enlarged grid size is set toward the outer boundaries. Calculation is started from an initial time step of (1.0 × 10⁻⁴) sand continuous until steady-state condition is reached. Solution in steady-state condition is checked by increasing the time step to show no dynamic response.

III. GEOMETRY & MESH GENERATION

The efficiency and accuracy of a numerical solution to explore the governing thermo-fluidic physics is highly dependent on the number and the distributions of the computational grid chosen. Furthermore, the stability and accuracy of such complex flow and heat transfer are highly dependent on the domain architecture and the grid structure. Meshes are generated using the Mesher tool available in the ANSYS WORKBENCH v16.0. Total number of cells and nodes are 42860 & 43538 respectively. The mesh arrangement used in the computational domain is shown in Fig. 1.2, where the full grid is displayed in Fig. 1.2(b) and close-up view near to the cylinder surfaces is present in Fig. 1.2(c).

IV. RESULTS

A. Thermo-Physical Properties of Micro-Flames for d=0.2mm

Simultaneous point measurements of temperature, major species (O₂, N₂, H₂O, and H₂), and OH concentrations are made in the radial direction at three axial locations (x = 0.1, 1, and 2 mm) of the micro-flames. Other quantities such as density and mixture fraction can be derived from the measured species concentrations. Figures 1.3–1.5 show the comparison of measured radial profiles of the mean temperature, major species (O₂, N₂, H₂O, and H₂), and OH concentrations with the calculated results using detailed reaction mechanisms for the d=0.2 mm flame. The measured mixture fractions (f) are also shown in the figures.
Figure 1.3 details the radial profile across the flame at $x = 0.1$ mm. The temperature rapidly rises from the centre of the jet to 1586 K, where it decreases across the reaction zone and then has a sudden drop across the flame edge. The $O_2$ and $N_2$ appear at the centre of the jet indicating leakage of ambient air into the flame. The maximum integrated $H_2$ intensity at the centre of the jet is only comparable to the intensity corresponding to the equivalence ratio ranges of $1.05 - 1.2$, which has a maximum equilibrium value of $H_2$ mole fraction of 0.065. The experimental uncertainties (15%, due to a small amount of $H_2$) may cause the measured mixture fraction to be slightly shifted to the lean side due to a large amount of $O_2$ and $N_2$ observed at the same location. The experimental uncertainty coupled with pre-heating enhanced thermal diffusion of $H_2$, and ambient air leakage could be the cause of no $H_2$ appearance around the centre of the micro-flames. Two OH peaks are found at the radial positions of $r = 0.35$ and $0.85$ mm. This indicates that two reaction zones are formed at this downstream location in the flame. The flame structure measured at this axial location contradicts to a general concept that only one reaction zone exists in a laminar hydrogen diffusion flame.

As the tube diameter is increased to 0.48 mm, comparisons of measured radial profiles of the mean temperature, major species ($O_2$, $N_2$, $H_2O$, and $H_2$), and OH concentrations with the calculated results are shown in Figs. 1.6–1.8 for $x = 0.1$, 1, and 2 mm, respectively. The distributions of temperature and species concentrations measured in this flame are similar to those observed in $d = 0.2$ mm flame at the same axial position except that the flame is larger. At $x = 0.1$ mm, the mean temperatures at the jet centreline ($T = 784$ K) and within the reaction zone ($T = 1680$ K) are higher than those of the $d = 0.2$ mm flame. The higher centreline temperature indicates significant heat loss from the flame to the entrained ambient air and the tube. Preheating of the entrained ambient air results in higher flame temperature & OH concentration. The OH distribution also indicates two reaction zones existing at this downstream position (Fig. 1.6).
Several important features are identified from the detailed measurements of micro flames. The coupled effect of air entrainment and disappearance of H$_2$ near the jet exit leads to lean-burn conditions for the flame (mixture fraction less than 0.0016). Moreover, the flame extends upstream of the burner port, suggesting that molecular diffusive-transport would dominate over the buoyant effect as here Richardson number (Ri) is much less than unity.

Again, observations & analysis are made on soot mass fraction along x=0.1, 1, 2 mm for d=0.2 & d=0.48 mm burner diameter& they are shown in Fig. 1.9 & Fig. 1.10.

It has been found out that for d=0.2 mm soot formation near the burner surface i.e. at x=0.1 mm is very less compared to at higher burner surface at x=2 mm & for d=0.48 mm soot formation is quiet high when compared with d=0.2 mm. In fig. 1.10 near burner surface at x= 0.1 mm soot formation rapidly increases up to 4.98 ppm at 1 mm radial distance & then decreases along the length.

Fig. 1.12: Comparisons of Contours of (a) Temperature Contour & (b) OH Mass Fraction Contour along the calculated Numerical Domain. Left Side is for d=0.2 mm & right side is for d=0.48 mm

V. CONCLUSION

In this report, Characteristics of micro-scale hydrogen diffusion flames produced from sub-millimetre diameter (d = 0.2 and 0.48 mm) tubes are numerically simulated using ANSYS FLUENT v16.0. Simultaneous, spatially and temporally point measurements are resolved of temperature, major species concentrations (O₂, N₂, H₂O, and H₂), and absolute hydroxyl radical concentration (OH) are made in the micro flames. It has been found that as ambient air leaks into the system therefore no H₂ molecules are detected at x =0.1 mm. The coupled effect of ambient air leakage and pre-heating enhanced thermal diffusion of H₂ leads to lean-burn conditions for the flame. Farther downstream (x = 1 and 2 mm), the temperature profiles become bell-shaped. The calculated characteristic features and properties indicate that the buoyancy effect is insignificant while the flames are in the convection–diffusion controlled regime because of low Peclet number. Also, the effect of Pe on the flame shape is insignificant as the flame is in the convection–diffusion controlled regime.

VI. NOMENCLATURE

1) d – Burner Diameter
2) Pe- Peclet number (~ u_e/μ)
3) u_e- Characteristic molecular diffusion velocity
4) u_m- Methane velocity at the needle exit
5) ω- Reaction Rate
6) ∇- Vector differential operator
7) ν- Kinematic Viscosity
8) T- Temperature
9) p- Dynamic Pressure
10) u- Velocity vector with radial (=r) & axial (=x) components
11) c_p- Heat capacity at constant pressure
12) λ- Thermal conductivity of fluid
13) ρ- Density of fluid
14) μ- Dynamic Viscosity
15) Y_i- Mass Fraction of i-th Species
16) z- Axial Direction
17) r- Radial Direction
18) q- Heat of formation per unit mass of methane/hydrogen
19) n_e- Stoichiometric coefficient based on mole for i-th species (n_f=1, n_o=2)
20) h- Flame Height
21) ν_v- Stoichiometric Coefficient of species based on mass (ν_v=4, ν_o=1)
22) g- Acceleration due to gravity

REFERENCES


