NUMERICAL PREDICTION OF FUEL DILUTION EFFECT ON THE FLAME STRUCTURE AND TEMPERATURE DISTRIBUTION IN DIFFUSION FLAME

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ABSTRACT

The techniques of dilution of fuel or air with inert gases such as nitrogen and argon are used to reduce pollutants in diffusion flame. The flame structure and the temperature distribution change significantly due to inert gas addition to fuel stream. In this work, a CFD code has been developed to predict the flame height and temperature distribution in an axisymmetric laminar confined methane-air diffusion flame after diluting the fuel with different percentages of nitrogen. The code is validated with the experimental results and the results obtained by running the CFD code are in well agreement with that of experimental results. The temperature of the air and fuel are initially taken as 300K. Mass flow rate of the fuel is taken as 3.71×10^{-6} kg/s and mass flow rate of the air is taken as 2.7103×10^{-6} kg/s. The total mass flow rate through the central jet (fuel jet) is, however, kept constant. The radiation effect is also included through an optically thin radiation model. An explicit finite difference technique has been adopted for the numerical solution of reacting flow. After grid independence test 85×41 grid nodes are finally adopted in which both accuracy of the results and the time of the program to run gets optimized. The code has been run on nitrogen dilution level of 0%, 20% and 50%. The flame height and temperature distribution are plotted against those dilution level. The prediction shows that flame height decreases with the addition of nitrogen to the fuel. Temperature of the flame is considerably reduced in the given computational domain.

Keywords: Methane, Laminar diffusion flame, Nitrogen dilution, Finite difference.

1. INTRODUCTION

Diffusion (non-premixed) flame is one of the most frequently used flames in practical combustion chambers like gas turbine combustors, internal combustion engines and industrial furnaces. The process of combustion is rather a highly complex phenomenon. According to Glassman [1], combustion simultaneously involves fluid mechanics, heat transfer and chemical kinetics. The analysis of the diffusion flame started with the flame sheet model due to Burke and Schumann [2]. Since then considerable progress has been made in understanding the diffusion flames. Experimental and numerical investigations of steady confined laminar diffusion flame were carried out by Mitchell et al. [3] to study the temperature, velocity and concentration profiles of stable species. Smooke et al. [4] obtained the numerical solution of the two-dimensional axi-symmetric laminar co-flowing jet

diffusion flame of methane and air both in the confined and the unconfined environment. Davis et al. [5] carried out a direct numerical simulation as well as the experimental verification of an unsteady low speed propane-air jet diffusion flame, utilizing the flame sheet and conserved variable approximations to investigate the dynamic structure of a buoyant jet diffusion flame.

A numerical simulation of an axi-symmetric confined diffusion flame formed between a H_2-N_2 jet and co-flowing air, each at a velocity of 30 cm/s, were presented by Ellzey et al. [6]. Katta et al. [7] developed a time dependent, axi-symmetric H_2-air diffusion flame model to study the effects of Lewis number and finite rate chemistry on the steady state and dynamic flame structures. Li et al. [8] investigated a highly over-ventilated laminar co-flow diffusion flame in axi-symmetric geometry considering unity Lewis number and the effects of buoyancy.

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Glassman [9] studied soot volume fractions and smoke heights of hydrocarbon fuels are postulated to be determined by the extent of incipient particle growth within co annular diffusion flames. Guo et al. [10] studied on thermal diffusion, caused by temperature gradients, tends to draw lighter molecules to warmer regions and to drive heavier molecules to cooler regions of a mixture. The influence of thermal diffusion on soot formation in co-flow laminar ethylene/air diffusion flames is numerically investigated in this paper. Chernovsky et al. [11] presented experimentally investigating fundamental characteristics of diffusion flames and the importance of gas radiation. In particular, transient measurements of flame growth, temperature, and radiation intensity of an expanding spherical diffusion flame in microgravity are used to investigate the effects of various diluents (nitrogen, carbon dioxide) with different radiative properties. Gillon et al. [12] have studied the behaviour of a laminar methane air flame with a central methane jet and a surrounding air co-flow and analysed that in a large range of fuel and air flow rates. In the present formulation, finite rate chemistry as well as the non-unity Lewis number and property variation have been considered. The radiation effect is also included through an optically thin radiation model. Recently, the natural gas is being used extensively for both stationary combustion system as well as vehicular application due to its eco-friendly nature as a fuel. Natural gas contains mainly methane and hence methane has been chosen as the fuel for the present study. Nitrogen is used as diluent in this work.

The combustion system considered is the laminar diffusion flame in a confined physical environment with coflowing fuel and air (oxidizer) streams. Two concentric vertical tubes comprise the burner. The fuel is admitted as a central jet through the inner tube and air as a co-flowing annular jet through the outer tube. The inner fuel tube diameter is 12.7 mm and the outer tube diameter is 50.4 mm. The inner tube wall is considered to be thin and its thickness is neglected for the computation. The dimensions are in conformity with the earlier experimental work of Mitchell et al. [3] and the numerical work of Smooke et al. [4]. The two streams diffuse into each other at the outlet of the inner tube in order to produce a flammable mixture of fuel and air. A cylindrical shield of diameter 50.4 mm defines an impervious outer boundary (wall) of the axisymmetric system. Considering the axi-symmetric geometry, the numerical simulations have been performed on one side of the axis only.

2. NUMERICAL MODEL

The combustion process is simulated with a detailed numerical model, solving the governing equations for reacting flow with appropriate boundary conditions. The flow is assumed to be laminar and axi-symmetric produced by a jet of fuel emerging from a circular nozzle, which burns in a co-flowing stream of air in a confined environment. Optically thin radiation model is considered here. Mass flow rate of fuel stream (methane

+ nitrogen) is kept constant in this work. Percentage of nitrogen is increased gradually to observe the difference. The reaction between the fuel and oxidizer proceeds through two-step irreversible chemical reactions. The flow is vertical through the reaction space and the gravity effect is included in the momentum equation. A variable property formulation has been made for the transport and thermodynamic properties. The model is shown in Fig. 1.
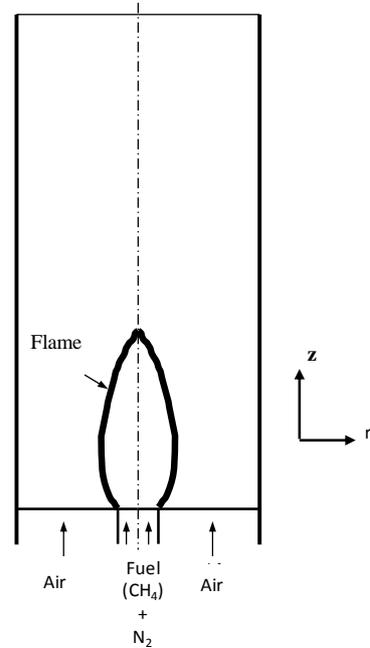

Fig.1. Physical Model of flame

3. GOVERNING EQUATIONS

The conservation equations considered here for mass and momentum in cylindrical co-ordinates are as follows:

Mass:

$$\frac{\partial \rho}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}(r\rho v_r) + \frac{\partial}{\partial z}(\rho v_z) = 0 \tag{1}$$
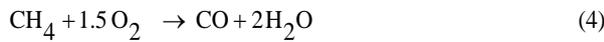
Radial Momentum:

$$\frac{\partial}{\partial t}(\rho v_r) + \frac{1}{r}\frac{\partial}{\partial r}\left(r\rho v_r^2\right) + \frac{\partial}{\partial z}\left(\rho v_r v_z\right) =$$

$$-\frac{\partial p}{\partial r} + \frac{2}{r}\frac{\partial}{\partial r}\left(r\mu\frac{\partial v_r}{\partial r}\right) - \frac{2}{r}\mu\frac{v_r}{r^2} +$$

$$\frac{\partial}{\partial z}\left\{\mu\left(\frac{\partial v_z}{\partial r} + \frac{\partial v_r}{\partial z}\right)\right\} -$$

$$\frac{2}{3}\frac{\partial}{\partial r}\left(\mu\left(\frac{\partial v_r}{\partial r} + \frac{v_r}{r} + \frac{\partial v_z}{\partial z}\right)\right) \tag{2}$$

Axial Momentum:

$$\frac{\partial}{\partial t}\left(\rho v_z\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\rho v_r\, v_z\right)+\frac{\partial}{\partial z}\left(\rho v_z^2\right)=$$

$$-\frac{\partial p}{\partial z}+\frac{1}{r}\frac{\partial}{\partial r}\left\{r\mu\left(\frac{\partial v_z}{\partial r}+\frac{\partial v_r}{\partial z}\right)\right\}$$

$$+2\frac{\partial}{\partial z}\left(\mu\frac{\partial v_z}{\partial z}\right)$$

$$-\frac{2}{3}\frac{\partial}{\partial z}\left\{\mu\left(\frac{\partial v_r}{\partial r}+\frac{v_r}{r}+\frac{\partial v_z}{\partial z}\right)\right\}+\rho g \qquad (3)$$

The combustion reaction of methane and air is assumed to proceed through simplified two-step global reaction chemistry as

$$CH_4+1.5O_2\;\rightarrow CO+2H_2O \qquad (4)$$

$$CO+0.5O_2\;\rightarrow\;CO_2 \qquad (5)$$

The reaction rates for the above reactions are obtained following an Arrhenius type rate equation, given as

$$\dot\omega = A\rho^{\left(\sum\limits_j a_j\right)}\frac{\prod\limits_j C_j^{a_j}}{\prod\limits_j M_j^{a_j}}\exp\left(-\frac{E}{\bar R\,T}\right) \qquad (6)$$

where, A and E are the pre-exponential factor and activation energy respectively for the respective equations and a_j is the reaction order in terms of jth reactant species. The values for these parameters are taken from the work of DuPont et al. [13].

The conservation equation for chemical species is solved for five gaseous species, viz. CH_4, O_2, CO_2, CO and H_2O. The concentration for N_2 is obtained by difference. The governing equation for the gaseous species conservation is as follows:

$$\frac{\partial}{\partial t}\left(\rho C_j\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\rho v_r C_j\right)$$

$$+\frac{\partial}{\partial z}\left(\rho v_z C_j\right)=\frac{1}{r}\frac{\partial}{\partial r}\left(r\rho D_{jm}\frac{\partial C_j}{\partial r}\right)$$

$$+\frac{\partial}{\partial z}\left(\rho D_{jm}\frac{\partial C_j}{\partial z}\right)+\dot S_{cj} \qquad (7)$$

where, C_j is the mass fraction of the respective species and D_{jm} is the diffusion coefficient of the species in a binary mixture of that species and nitrogen (following

Katta et al., [7]). The source term $\dot S_{cj}$ is the rate of production or destruction of the species j per unit volume due to chemical reaction.
The source terms are calculated as

$$\dot S_{cj}=\sum_{k=1}^{2}\left(\gamma''_{jk}\dot\omega_k-\gamma'_{jk}\dot\omega_k\right)M_j \qquad (8)$$

where, M_j is the molecular weight of the jth species. γ''_{jk} and γ'_{jk} are the stoichiometric coefficients on the product side and reactant side respectively for the jth species in the kth reaction. Obviously, for the present simple reaction mechanism, k is either 1 for the reaction given by Eq. (4) or 2 for the reaction given by Eq. (5).

$$h=\sum_{j=1}^{n}C_j h_j=\sum_{j=1}^{n}C_j\left(h_{fj}^0+\int_{T_0}^{T}c_{pj}dT\right) \qquad (9)$$

The density of the species mixture is calculated using the equation of state considering all the species as ideal gases. The enthalpy for chemically reacting flow is given as the weighted sum of each mass fraction according to the following relation: where, h_{fj}^0 is the heat of formation of the jth species at the reference temperature T_0 and the integral part is the contribution of the sensible heat.

The energy equation is written as

$$\frac{\partial}{\partial t}\left(\rho h\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\rho v_r h\right)+\frac{\partial}{\partial z}\left(\rho v_z h\right)$$

$$=\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\lambda}{c_p}\frac{\partial h}{\partial r}\right)+\frac{\partial}{\partial z}\left(\frac{\lambda}{c_p}\frac{\partial h}{\partial z}\right)$$

$$-\frac{1}{r}\frac{\partial}{\partial r}\left(rq_{R_r}''\right)-\frac{\partial}{\partial z}\left(q_{R_z}''\right)$$

$$+\frac{1}{r}\frac{\partial}{\partial r}\left[r\frac{\lambda}{c_p}\sum_{j=1}^{n}h_j\left(Le_j^{-1}-1\right)\frac{\partial C_j}{\partial r}\right]$$

$$+\frac{\partial}{\partial z}\left[\frac{\lambda}{c_p}\sum_{j=1}^{n}h_j\left(Le_j^{-1}-1\right)\frac{\partial C_j}{\partial z}\right] \qquad (10)$$

q_{R_r}'' and q_{R_z}'' represent the r and z components of the radiative heat flux respectively. Lej in the above equation is the local Lewis number of the jth species defined as

$$Le_j=\frac{\lambda}{c_p}\frac{1}{\rho D_{jm}} \qquad (11)$$

The last two terms in the energy equation, i.e., Eq. (10) are caused by the preferential diffusion of species in the radial and axial directions respectively. The specific heat c_p is a strong function of temperature and is locally calculated for each species at the respective temperature. The mixture specific heat is then calculated considering an ideal gas mixture. The temperature of the gas mixture is implicitly calculated by solving Eq. (9) using Newton-Raphson method. The solution is refined until the accuracy within the prescribed criteria (i.e. 0.003%) is achieved.

The transport of momentum, energy and species mass in the calculation of a reacting flow involve the transport coefficients like viscosity (μ), thermal conductivity (λ) and mass diffusivity (D_{jm}) for the solution. The local viscosity of the species j is computed from the local temperature using a power law as,

$$\mu_j = \mu_j^0 \left(\frac{T}{T_0} \right)^p \qquad (12)$$

μ_j^0 represents the reference viscosity of species j at the reference temperature T_0. The power exponent p is taken as 0.7, in conformity with the earlier work of Smooke et al. [4]. The viscosity of the mixture is calculated using the semi-empirical method of Wilke, as described in Reid et al. [14].

The local thermal conductivity of species j is evaluated using a polynomial expression of thermal conductivity of pure substance as

$$\lambda_j = A_j + B_j T + C_j T^2 + D_j T^3 \qquad (13)$$

where, Aj, Bj, Cj, and Dj are the coefficients for species j, which are taken from Reid et al., [14]. The mixture thermal conductivity is again evaluated using the method of Wilke.

Specific heat of the species c_{pj} is a function of temperature

$$c_{pj} = a_j + b_j T + c_j T^2 + d_j T^3 \qquad (14)$$

Values of co-efficient are taken from Reid et al., [14]. The mass diffusivity, D_{jm}, for species j in a binary mixture of j and nitrogen is evaluated using a power law (Turns, [15]) as

$$D_{jm} = D_{jm}^0 \left(\frac{T}{T_0} \right)^{1.5} \qquad (15)$$

The variation of thermodynamic and thransport properties with temperature has been taken care of by fitting suitable polynomials and correlations over the entire temperature range. The details of this formulation can be obtained from the previous work of Mandal et al. [16]. An optically thin radiation model as described by Datta and Saha [17] has also been included in this formulation.

4. BOUNDARY CONDITIONS

Boundary conditions at the inlet are given separately for the fuel stream at the central jet and the air stream at the annular co-flow. The fuel jet is a mixture of methane and nitrogen. The amount of nitrogen in the fuel jet is denoted by nfrac and this is supplied as input. The streams are considered to enter the computational domain as plug flow, with velocities calculated from their respective flow rates. The temperatures of both fuel and air at inlet are taken as 300 K. In conformation with the conditions used by Mitchell et al. [3], and Smooke et al. [4], the fuel flow rate is taken as 3.71×10^{-6} kg/s and the air flow rate is taken as 2.2104×10^{-4} kg/s. Considering the length of the computational domain to be 0.3 m, the fully developed boundary conditions for the variables are considered at the outlet. In case of reverse flow at the outlet plane, which occurs in the case of buoyant flame, the stream coming in from the outside is considered to be ambient air. Axi-symmetric condition is considered at the central axis, while at the wall a no-slip, adiabatic and impermeable boundary condition is adopted.

5. SOLUTION METHODOLOGY

The gas phase conservation equations of mass, momentum and energy and species are solved simultaneously, with their appropriate boundary conditions, by an explicit finite difference computing technique. The solution yields velocity, temperature, and species concentration. The numerical scheme adopted for solving the reacting flow problem is based on a straight-forward, yet powerful algorithm called SOLA (Solution Algorithm) developed by Hirt and Cook [18]. The algorithm is based on primitive variables and the variables are defined following a staggered grid arrangement (Fig. 2). The axial and radial components of velocity (v_z and v_r) are defined at the scalar cell faces while the scalar properties (pressure, temperature, species concentration), the fluid properties (density, viscosity and specific heat) and the source terms (volumetric rates of heat generation and species,) are defined at the centers of the cells. The solution is explicitly advanced in time till a steady state convergence is achieved.

5.1 Grid Size

A variable size adaptive grid system is considered An extensive grid independence test is carried out by several variations of the number of grids in either direction. It is observed that the increase in the numbers of grids from 85×41 to 121×61 almost doubles the computation time, but the maximum change in results is within 2%. Hence a numerical mesh with 85×41 grid nodes is finally adopted.

5.2 Discretization Scheme

The transient transport equations are discretized using explicit finite differencing technique. The diffusion terms are discretized by a central differencing scheme, whereas the advection terms are discretized by a hybrid

differencing schemes as described by Patankar [19]. The source terms are considered to be constant throughout the volume of each cell.

5.3 Ignition

The ignition of the fuel-air mixture in the combustion chamber is simulated by raising the temperature of the mixture within a few cells, to 1000 K, near the fuel-air interface (slightly above the burner tip) and maintaining it there till the local temperature of the flammable mixture is raised beyond the ignition temperature due to reaction. This is achieved by adding a heat source of suitable value in such a way that the combustion sustains and also remains within the control. The location of ignition (i.e. heat source addition points) is chosen considering the fact that the concentration ratio of the fuel and air in the corresponding cells remains within the flammability limit.
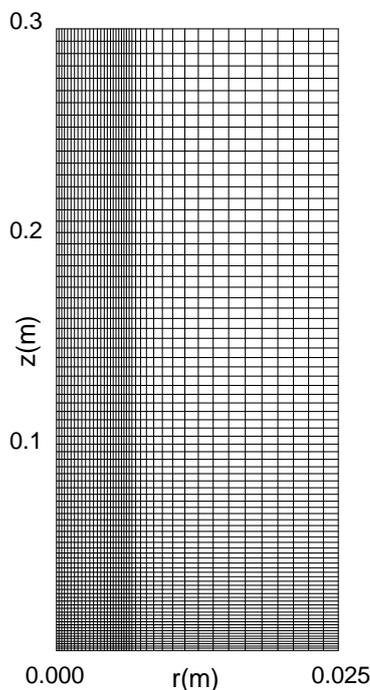
simulated with fuel diluted by adding nitrogen to it. The fuel is diluted by adding 20% and 50% of nitrogen and also without dilution (0 %) keeping the total mass flow rate of the fuel stream (methane + nitrogen) at the same value 3.71×10^{-6} kg/s. The fuel is diluted by adding 0% (no dilution), 20% and 50% of nitrogen by mass respectively. The fuel is diluted by adding 20% and 50% of nitrogen keeping the total mass flow rate of the fuel stream (methane + nitrogen) at the same value 3.71×10^{-6} kg/s. The numerical results are post processed to obtain flame shapes for the above two cases. The temperature distributions have also been presented for no dilution (0% nitrogen) and dilution with 20% and 50% nitrogen cases. The flame front is described by the volumetric heat release rate contour having value 1% of the maximum local volumetric heat release rate due to chemical reaction.
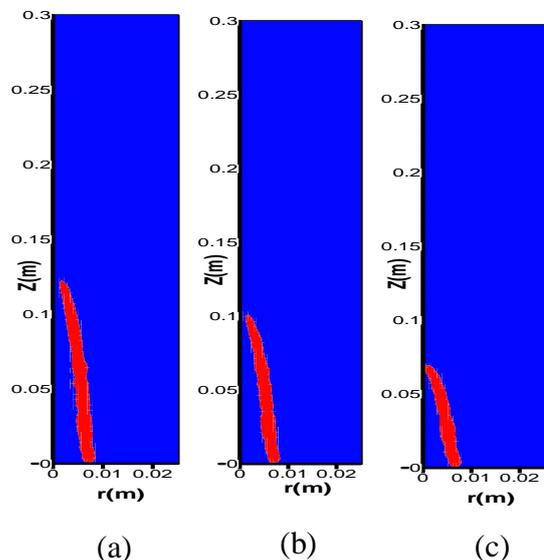

Fig.2. Grid Structure

(a)   (b)   (c)

Figure 3 Shape of the flame fronts for different nitrogen dilution: (a) 0% (b) 20% (c) 50%

The flame front is described by the volumetric heat release rate contour having value 1% of the maximum reaction. Figure 3(a) to (c) shows the flame shape. It may be noted from the figure that the flame height reduces progressively as dilution is increased.

Figures 4(a) to 4(c) show the temperature distributions throughout the computational domain for three dilution cases as described earlier. It is observed that the peak temperature zone height is lowered as the dilution level increases. This also confirms the lowering of flame height with dilution. Maximum value of temperature is decreasing with the increase of nitrogen dilution.

Temperature around the wall throughout the computational domain is less than 400 K. Due to dilution the temperature of the different species in the computational domain decreases. The temperature along the centerline is increasing in every case of dilution and without dilution. But height of maximum temperature is decreasing with increase of dilution.

6. RESULTS AND DISCUSSION

A numerical code on computational fluid dynamics and heat transfer can only be accepted if results obtained from the simulation of the code match quite well with the experimental results under similar condition available in the literature or the results obtained from side by side experiments. The numerical code for the reacting flow is validated by comparing the predictions against experiments conducted by Mitchell et al. [3] within the flame for the same input and operating conditions. The model is validated against the experimental and numerical results of Smooke et al. [19] under no dilution condition. The results show good agreement with the experiments. The laminar confined axisymmetric co-flow methane/air diffusion flame is
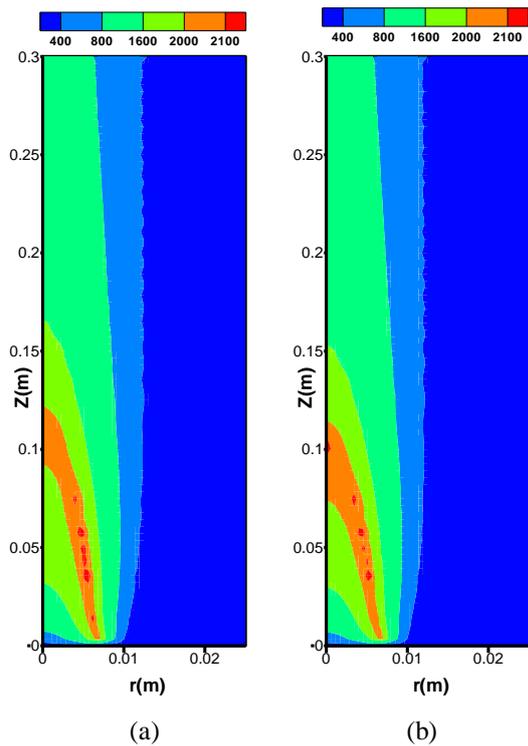
(a)   (b)

(c)

Figure 4 Temperature (in K) Distributions for different nitrogen dilution: (a) 0% (b) 20% (c) 50%

When nitrogen is added with methane with increasing percentage, the height at which peak value of bulk mean temperature occurs gets decreased gradually. Bulk mean temperature variation in the centerline is shown in Figure 5. Bulk mean temperature is increasing up to a height of 8 cm for the case when nitrogen is not added to methane at the centreline.
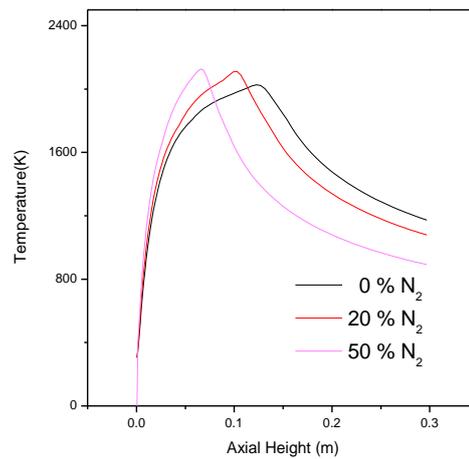

Figure 5 Centerline temperatures at different dilution level of CH_4 with nitrogen

7. CONCLUSIONS

A numerical study on a laminar axisymmetric coflow methane air diffusion flame in a confined environment without nitrogen and also with different nitrogen dilution level up to 50% dilution has been carried out. Different conservation equation for mass, axial momentum, radial momentum and energy are solved using two step equations by finite differencing technique. The temperature and flame height are analyzed in different dilution levels. Soot properties such as the diameter, volume fraction and the number density of soot are also presented in this study. The flame height is found to be around 12 cm without dilution and it reduces with the increase of percentage of nitrogen to methane and becomes approximately 7 cm when nitrogen in the mixture is 50 %.The flame also flattens out in radial direction for higher dilution levels. This gives rise to a near spherical flame shape as dilution level increases. The peak temperature decreases with the increase of dilution. It is around 2200K without dilution and decreasing gradually with different dilution. High temperature zone is limited to a small distance in the radial direction in case of comparatively higher dilution levels.

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NOMENCLATURE

a_j	=Reaction order with respect to jth species	
C_j	= Concentration of the jth species	
c_P	= Specific heat	$J.kg^{-1}.K^{-1}$
D	= Mass diffusivity	$m^2.s^{-1}$
g	= Acceleration due to gravity	$m.s^{-2}$
h	= Enthalpy	$J.kg^{-1}$
Le	=Lewis number	
p	= Pressure	bar
r	= Radial distance	m
T	= Temperature	K
t	=Time	s
v	= Velocity	$m.s^{-1}$
z	= Axial distance	m

Greek Symbols

μ	= Viscosity	$kg.m^{-1}.s^{-1}$
ρ	=Density	$kg.m^{-3}$
λ	= Thermal conductivity	$W.m^{-1}.K^{-1}$

Subscript

j	= Species identification
r	= Radial direction
z	= Axial direction

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