Measurements of Flame Temperature of Energetic Gaseous Fuels using Sodium Line Reversal Technique and Emission Spectroscopy

N. Tiwari[1], S. N. Sahasrabudhe[1], A. K. Tak[1], P.V. A. Padmanabhan[1], A. K. Das[1],V. S. Prabhakar[2],
P. C. Palwankar[2], S. Tyagi[2], P. V .C Rao[2]
[1]Laser and Plasma Technology Division, BARC
[2]Bharat Petroleum Corporation Ltd
Trombay,Mumbai, Maharashtra - 400085 ,
India.

Abstract - **A new fuel with some additives to LPG is developed by Bharat Petroleum Corporation Limited for metal cutting application. This is a cheaper substitute for Acetylene and is named as Bharat Metal Cutting Gas (BMCG). We have measured temperature in the flame produced by Oxy-BMCG and Oxy-LPG flames in a brazing torch. Sodium line reversal method was used to measure temperature in secondary flame region and Boltzmann plot method was used to measure temperature in bright primary flame, near to the torch nozzle. Under similar conditions, temperature of Oxy-BMCG flame is higher than that of Oxy-LPG flames by about 50 to 120^{0}C in primary flame region and about 250 to 350^{0}C in secondary flame region. The highest temperature zone of the flame was found to lie closer to the primary flame. A CFD simulation to get the flame temperature has been done and the results are compared with the experimental results. The technique can be used by fuel scientists for their routine evaluation of high energy fuels.**

Keywords: Sodium Line Reversal, Emission Spectroscopy, Temperature Measurement

1. INTRODUCTION:

Metal cutting in the industries is routinely done by oxy-acetylene flames. These flames produce temperatures up to about 3800 K. The fuel gas industry is constantly endeavoring to replace oxy-acetylene by cheaper alternative like liquefied petroleum gas (LPG). However, the temperature of oxy-LPG flame is only about 2800 K, which is less than that required for metal cutting. M/s. Bharat Petroleum Corporation Ltd has developed a viable alternative to acetylene by introducing additives to LPG, which is called Bharat Metal Cutting Gas (BMCG). Temperature of oxy-BMCG flame is higher than that of oxy-LPG flame and has been found to be suitable for metal cutting applications. The present paper reports characterization of the BMCG and LPG fuels with respect to flame temperature. Centerline temperature of the oxy-LPG flame was measured at various distances from the nozzle by Sodium line reversal technique. Very near the exit of nozzle, a bright light blue primary flame results. This is due to a transition near to 431.5 nm due to excited C-H radical. Temperature of this part of the flame was determined by Boltzmann plot method. With these data, the temperature in the oxy-LPG flame was mapped.

Sodium line reversal is a standard technique for measurement of temperature in flames produced by fuels like LPG, acetylene etc[1,2]. In this technique, light from a black body of known temperature is passed through the flame seeded with a sodium salt. When the temperature of the black body is higher than the temperature of the flame, the spectrum of the light passing through the flame shows dips at the sodium lines with wavelengths 589 and 589.6 nm. The temperature at which the 'dip' just starts appearing gives the temperature of the flame. This technique is explained in some details in the next section. This is a useful method to determine flame temperature below 2800 K.

2. EXPERIMENTAL METHODS:

Oxy-LPG or oxy-BMCG flame was produced using a commonly used oxy-Acetylene brazing torch. The torch was mounted vertically with flame directed upwards. Nozzle of the torch is made of copper and has internal diameter (ID) of 1 mm. A mixture of fuel and oxygen was used to produce the flame. Fuel and oxygen flow rates were controlled by rotameters. Resulting flame length varied from about 10 cm to 25 cm depending on flow rates. The flame thus produced has two parts a primary flame near the nozzle and a secondary flame as shown in Fig.1

Region where the temperature is less than 2800 K determined by Sodium line reversal.

Faint blue secondary flame

Highest temperature zone

Bright blue primary flame. Temperature by emission spectroscopy.
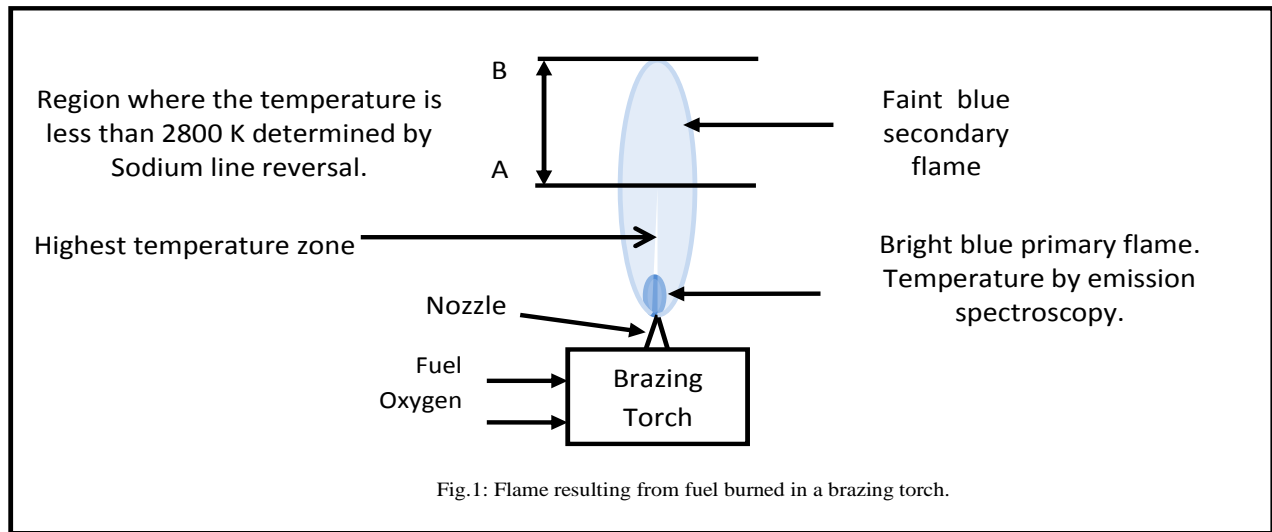
Nozzle

Fuel
Oxygen

Brazing Torch

Fig.1: Flame resulting from fuel burned in a brazing torch.

Very near to the nozzle, partial oxidation of the fuel takes place and the excited C-H radicals are present in high concentration. The C-H radical has emission line at 431.5 nm giving a bright blue color to the primary flame. The secondary flame is the portion where the rest of the fuel is oxidized. The flame expands in radial and axial directions, becomes faint and eventually merges with the cold surrounding. Primary flame is bright enough for emission spectroscopy and temperature can be determined by Boltzmann plot method using rotational lines around the 431.5 nm [3,4]. Secondary flame is very faint and emission spectroscopy without ICCD (or similar) detector is not possible. The temperature of the secondary flame was determined by Sodium line reversal method [2]. This method can determine temperature up to 2800 K. Temperature of the secondary flame varies from the nozzle to the tip. At the tip of the flame, the temperature may be close to 1800 K (Point B in Fig.1) and it exceeds 2800 K (Point A, in Fig.1). Temperature in the region between the

nozzle and point A, is higher than 2800 K and cannot be measured by line reversal technique. The data near the tip is then extrapolated to estimate the flame temperature in this region.

2.1 Sodium line reversal technique:

This is a standard technique based on the principle of Fraunhofer lines found in emission spectrum of the Sun. The principle is explained in Fig. 2. A Black body source is seen by a spectrograph through the flame seeded with sodium. When the temperature of the black body is less than that of the flame, sodium lines appear brighter than the background, $T_{BB} < T_F$, as shown in Figure 2. When both the temperatures are equal, the lines merge with the surroundings, $T_{BB} = T_F$ as shown in Fig.2. When the black body temperature is more than that of the flame, the lines appear darker compared to the background, $T_{BB} > T_F$ as shown in Fig.2

Black body radiation source

Flame

Spectrograph

O/P of spectrograph

Light beam

Sodium Seed

$T_{BB} < T_F$

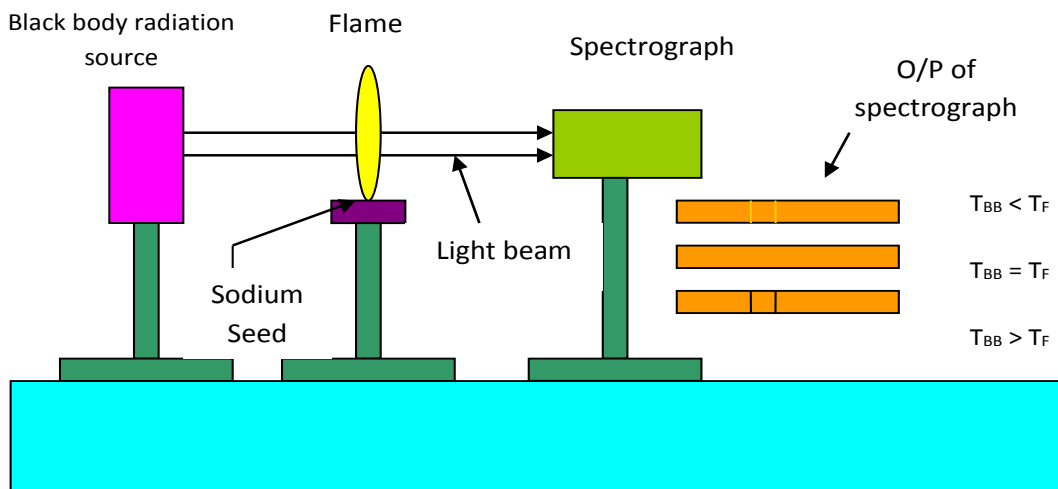$T_{BB} = T_F$

$T_{BB} > T_F$

Fig. 2: Line reversal technique: schematic of experimental arrangement

A calibrated tungsten strip lamp was used as a black body source and a spectrograph (model: Shamrock 303i) with CCD (model: Andor 420A) was used as the detector. The black body spectrum and sodium line spectrum together was recorded by the spectrograph on real time basis. When the black body temperature was increased slowly, we observed the sodium line merging into the background and eventually the reversal was observed. We noted the temperature at which the sodium lines merged with the background as the flame temperature. Only the center line temperature of the flame was measured.

2.2 Spectroscopic Technique:

The relative line intensities of emission lines of the hot gas in thermodynamic equilibrium depend on its temperature. Relative line intensities are related by Boltzmann relation. The rotational lines also obey this relation. The rotational band around 431.5 nm line emitted by the C-H* radical in $A^2\Delta \to X^2\Pi(0,0)$ transition consists of several rotational lines . The rotational temperature is very close to the translational temperature [5]. A spectrograph having resolution better than 0.02 nm can be used to get these line intensities of rotational lines with very close wavelengths

(~0.2 nm) and with Boltzmann plot one can get the temperature of the hot gas. The temperature of primary flame of LPG and BMCG was determined by this method. Experimental system is shown in Fig. 3 and the typical spectrum around 431.5 nm is shown in Fig. 4. This technique is based on the measurement of the intensity of spectral lines in vibration-rotation band of chemical species, in this case, the radical CH*. The relation between the line intensity (I) and the temperature (T) for a specific transition is given by the equation

$$I = CS_{J'J''}\lambda^{-4}\exp(-E_{J'}/kT)$$

In the above equation, $S_{J'J''}$ is the line strength of a transition from the upper (J') to the lower (J'') rotational state; $E_{J'}$ is energy of the upper rotational level and C a constant. If the system shows Boltzmann distribution, a plot of the natural logarithm of line intensities versus energy of the exited level is a straight line, whose slope is the inverse of the rotational temperature.
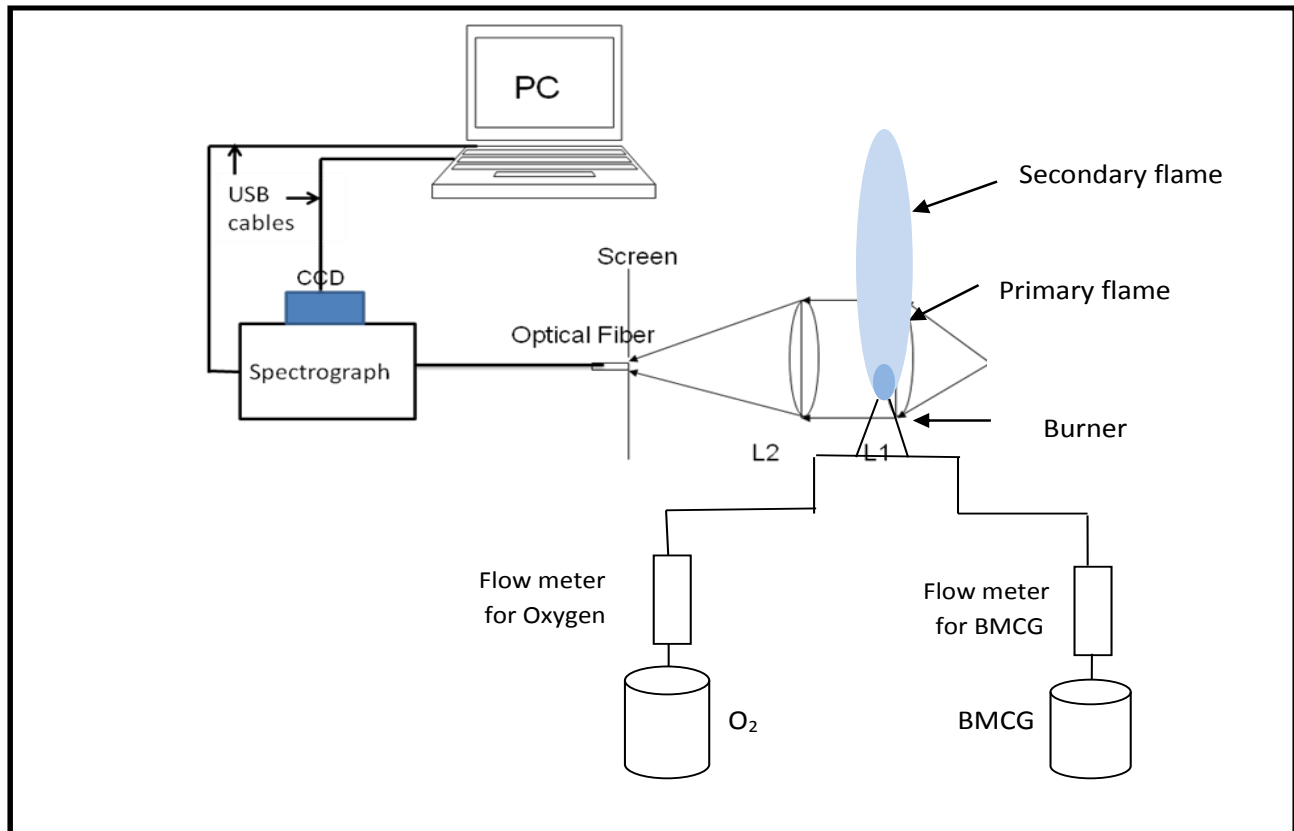

Fig. 3: Experimental setup for spectroscopic determination of primary flame temperature.

Flames were produced from a gaseous mixture of LPG or BMCG and oxygen. LPG is a mixture of propane + butane. Fuel flow and oxidizer flow were controlled by calibrated flow meters. Spectrum in the range of 400 to 440 nm

corresponds to the rotational band of $A^2\Delta \to X^2\Pi(0,0)$ transitions around 431.5 nm. The emission spectrum obtained at 1mm from nozzle exit is shown in Fig.4.
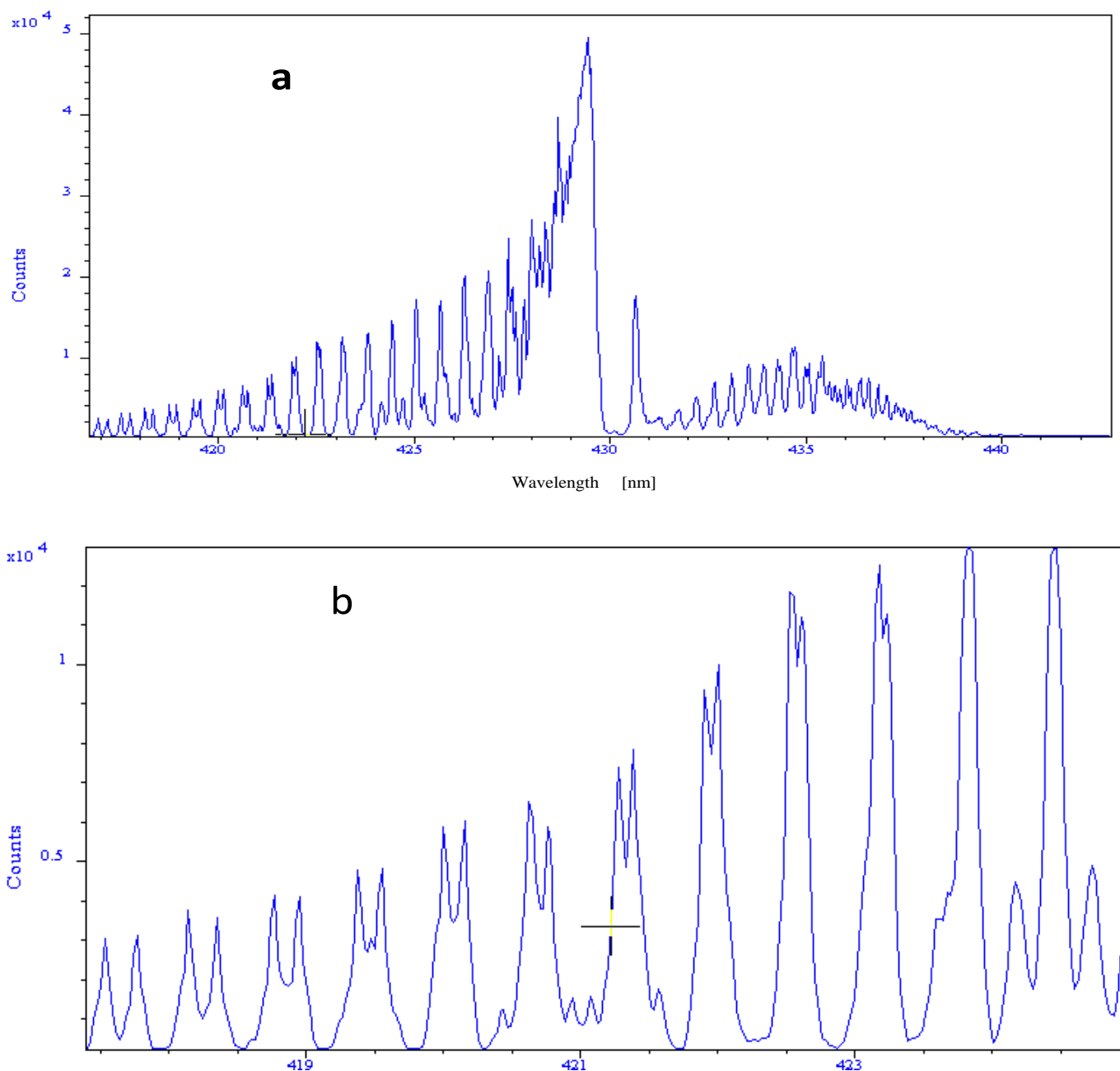
Fig. 4: a) Typical vibration-rotation band around 431.5 nm b) Expanded view of rotation spectrum

CH* emission spectra show an intensity maximum, at 431.5 nm. In this region, there is an overlapping of the 0-0 and 1-1 vibrational bands, as well as an isolated peak at 432.4 nm, which corresponds to the 2-2 band. The spectral range between 416 and 425 nm is predominantly the R-branch of the 0-0 band, with J value from 11 to 20. For $J \geq 7$ this branch shows a rotational structure sufficiently spaced with no interference from other peaks and therefore is suitable for intensity measurements. This region, which appears as doublet peak, was used for rotational temperature determination by the Boltzmann plot method. The spectral lines taken for the analysis were identified in the above figure. Area under the curve for each wavelength was calculated. Plot of natural logarithm of the experimentally measured relative intensities $\ln(I\lambda^4 /S_{J'J''})$ Vs $-(E_{rot}/k_BT)$ is a straight line, and the slope of the line gives the temperature. Typical Boltzmann plots are shown in Fig. 5
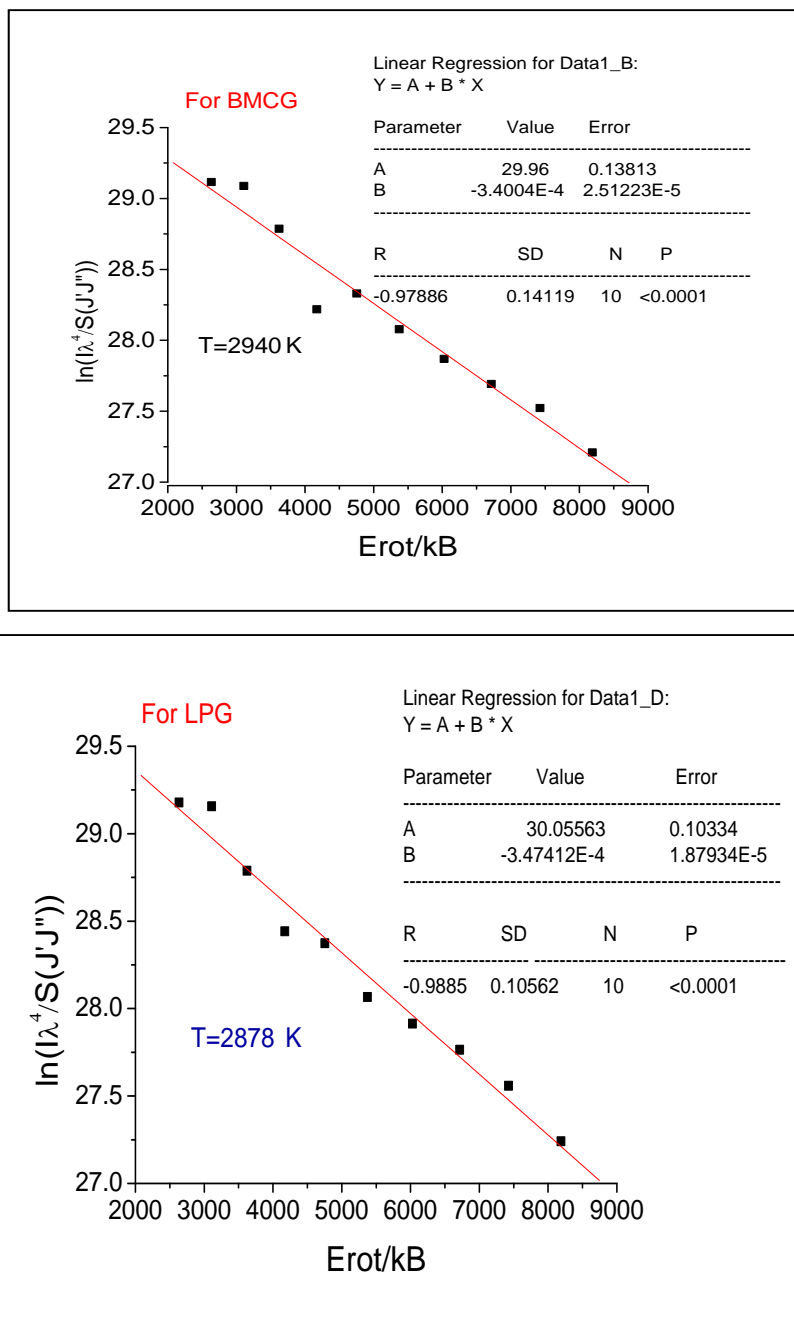
Fig. 5: Typical Boltzmann plot for CH* rotational spectrum for BMCG for LPG flames. (Temperatures: 2940 K and 2878 K respectively)

3. EXPERIMENTAL SYSTEM AND PROCEDURE

3.1 Stoichiometry: Three sets of measurements with LPG and BMCG at flow rates of 0.1, 0.14 and 0.18 SLM were carried out. Oxygen at stoichiometry is 6.5 times by volume of LPG assuming LPG and BMCG have chemical composition of C_4H_{10}. The oxidation reaction for complete burning of butane is given below:

$$C_4 H_{10} + 6.5 \, O_2 = 4 \, CO_2 + 5 \, H_2O$$
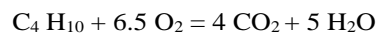
Appropriate flow rate of oxygen and fuel for stoichiometric oxidation was ensured by visual observation of the flame properties. Oxygen flow was slowly increased till the luminous portion due to hot carbon particles in the flame just disappeared indicating that the oxygen supply was just stoichiometric. This is the flame which can be called as 'just oxidizing' flame. The flame length of BMCG was observed to be longer than that of LPG flame for the same volume flow rate.

3.2 Secondary flame temperature:

The tungsten strip lamp was calibrated with a two color pyrometer. Temperature of the filament was calibrated against current flowing through the lamp. Fuel gas flow rates were adjusted at 0.1, 0.14 and 0.18 SLM for three sets of readings for LPG and BMCG. Oxygen flow rate was regulated to stoichiometry. Temperature measurement was carried out exactly along the axis of the flame. For this, the brazing torch was mounted on a X-Y-Z table and its nozzle axis was aligned exactly perpendicular to the optical axis of lenses used in the setup as shown in Fig. 6. Sodium seeding was done by introducing a thin SS rod dipped in sodium carbonate (Na_2CO_3) into the flame near the nozzle. In order to ensure minimum disturbance of the flame by sodium seeding the amount of seeding was controlled so that the intensity of sodium lines corresponded to 1000 to 1200 counts on the CCD of the spectrograph. Extensive trial experiments were carried out to arrive at the minimum concentration of sodium required to observe the reversal without disturbing the flame. The spectrograph shows the continuum signal from the tungsten strip lamp and sodium D1 & D2 lines at 589 and 589.6 nm under real time operation mode i.e. the data was updated in about a second. A low resolution grating (300 lines/mm) was used to see the continuum signal and the sodium lines together. This arrangement was adequate for observing the point of line reversal but has the disadvantage of not resolving the two sodium lines. The two sodium lines are seen as a single peak without the tungsten lamp ON in Fig. 7(a) and the sodium lines (single peak) are seen riding over the continuum in Fig. 7(b). Fig. 7(c) shows that the continuum intensity has increased with the sodium lines merged in the background. With further increase in the continuum intensity (Fig. 7d), the sodium lines appear as a dip indicating the reversal.
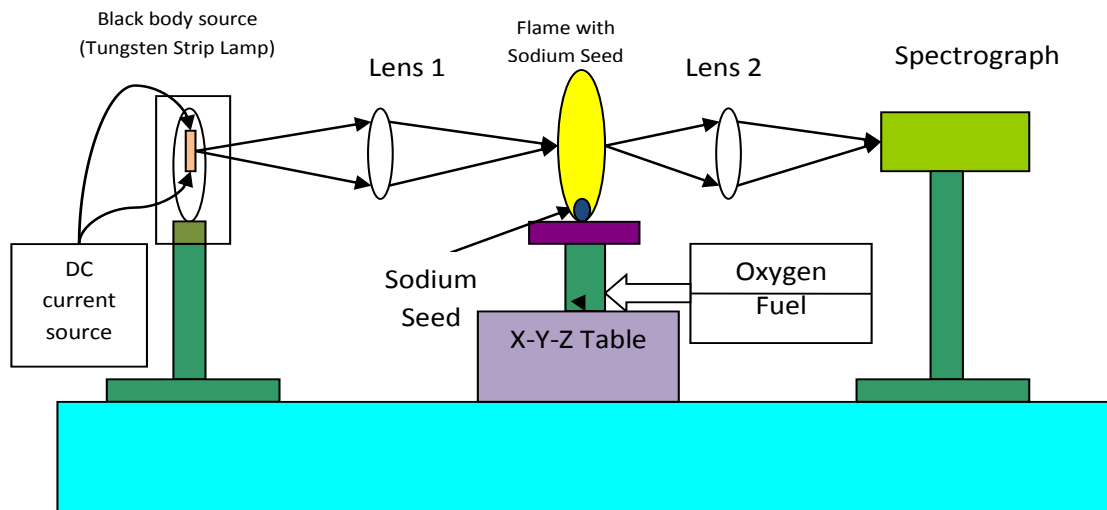

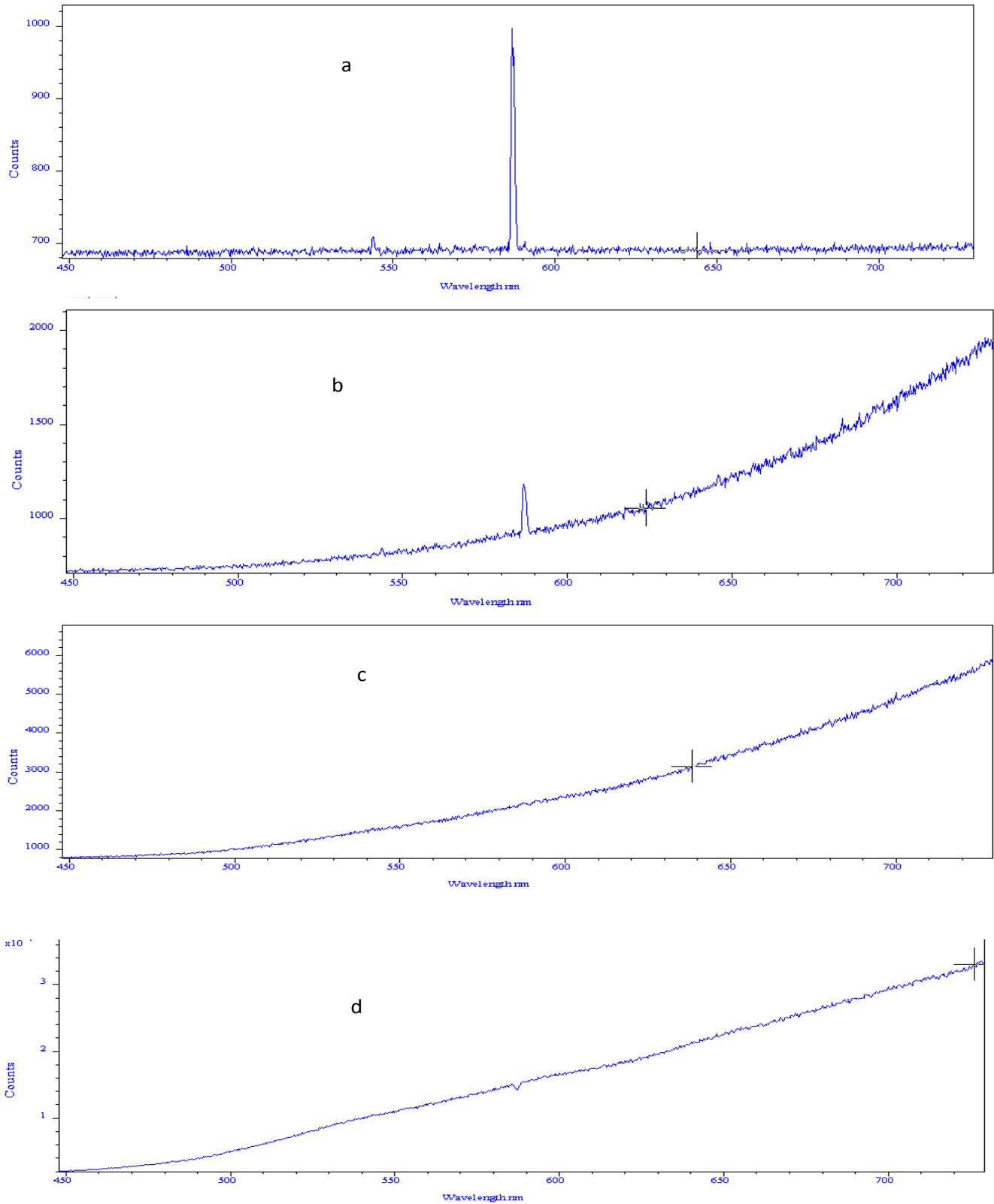Fig. 6: Experimental set up of flame temperature measurement by line reversal technique

Fig. 7: a) Sodium line and without continuum background of the lamp. b) Sodium line and the continuum background of the lamp. One can see the sodium line riding over the continuum. (With filament current 9 A).c) Sodium line merging into the continuum background of the lamp. (With filament current 12 A). d) Sodium line is seen as a Fraunhofer line against brighter continuum background (a dip) of the lamp. This is the line reversal.(Filament current > 15A)

Fuel flow rates of 0.1 SLM, 0.14 SLM and 0.18 SLM were used to produce the flame. Increasing the fuel flow rate was seen to increase the length of the flame. Fuel flow rate higher than 0.18 SLM was not used because the range of the X-Y-Z table was not sufficient to scan the flame beyond the fuel flow rate of 0.18 SLM. It was observed that the flame length with BMCG was much longer than that for the same flow rate of LPG.

3.3 Primary flame temperature:
Determination of primary flame temperature has been carried out by spectroscopic technique based on the principle discussed under section 2.2. Lenses were adjusted in such a way that they focus the bright primary flame on to the optical fiber and collect the spectral data. A grating of 2400 lines/mm was used to get higher spectral resolution. However, for resolving rotational lines, which are very close the resolution of this grating is not adequate. A higher resolution grating, which gives a resolution of better than 0.02 nm would be ideal for the spectroscopic measurement of primary flame temperature. The exposure time for collecting data was kept about 10 seconds in order to get good signal to noise ratio. Slight error in the calculation of intensity (i.e area under the curve with a proper base for one spectral line) is reduced when logarithm of the intensity is taken in the equation for Boltzmann Plot.

4. MODELING AND SIMULATION

Fluid dynamic simulation has been carried out to calculate flame temperatures and the simulation results have been compared with experimentally measured temperature data. Enthalpy of reaction was taken into account using a simplified model in which chemical reaction was replaced by an appropriate heat source. Complete combustion of butane was assumed. A cylindrical zone of 4 mm diameter and 15 mm length was assumed as a uniform heat source. Heat of combustion was taken to be 2.38 KW per SLPM of butane .The conservation equations for various quantities such as energy, mass, momentum, turbulent kinetic energy and its dissipation rate etc. can be written in the generalized form suggested by Patankar[6]. Here, ϕ represents the scalar quantity for which the conservation equation is to be solved, ρ is the fluid mass density, V the velocity vector, Γ_ϕ the diffusion coefficient for the scalar, S_ϕ the source term. While solving for energy and momentum conservation equations, ϕ is replaced by T, the temperature, u, v the Cartesian components of velocity respectively. The various quantities for which the conservation equations are solved for a three dimensional system are presented in table 1.

$$\vec{\nabla} \cdot (\rho \upsilon \vec{\phi}) = \vec{\nabla} \cdot (\Gamma_\phi \ \vec{\nabla}_\phi) + S_\phi. \qquad (1)$$

Conservation Quantity	Conservation Equation	
Mass	$\frac{\partial \rho}{\partial t} + \text{div}(\rho \boldsymbol{u}) = 0$	(2)
X momentum		
Y momentum	$\frac{\partial(\rho u)}{\partial t} + \text{div}(\rho u \boldsymbol{u}) = -\frac{\partial p}{\partial x} + \text{div}(\mu \text{ grad } u) + S_{Mx}$	(3)
Energy	$\frac{\partial(\rho v)}{\partial t} + \text{div}(\rho v \boldsymbol{u}) = -\frac{\partial p}{\partial y} + \text{div}(\mu \text{ grad } v) + S_{My}$	(4)
	$\frac{\partial(\rho i)}{\partial t} + \text{div}(\rho i \boldsymbol{u}) - \text{p div } \boldsymbol{u} + \text{div}(k \text{ grad } T) + \Phi + S_i$	(5)

In equations (2)–(5), u, μ, κ, C_P, ϕ are, respectively, the velocity vector, the viscosity, the thermal conductivity, and specific heat of the gas and dissipation function due to viscous stresses. The thermodynamic and transport properties depend on the local temperature. P represents the pressure. Computational domain and the mesh is shown in figure 8 given below.
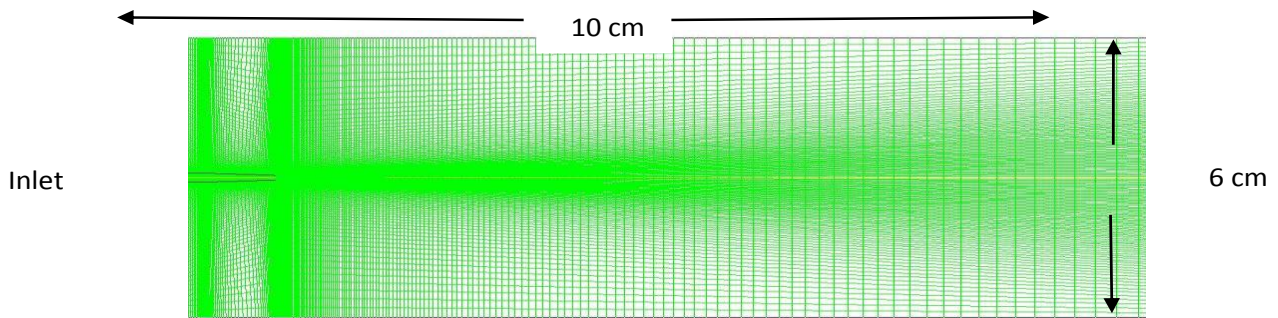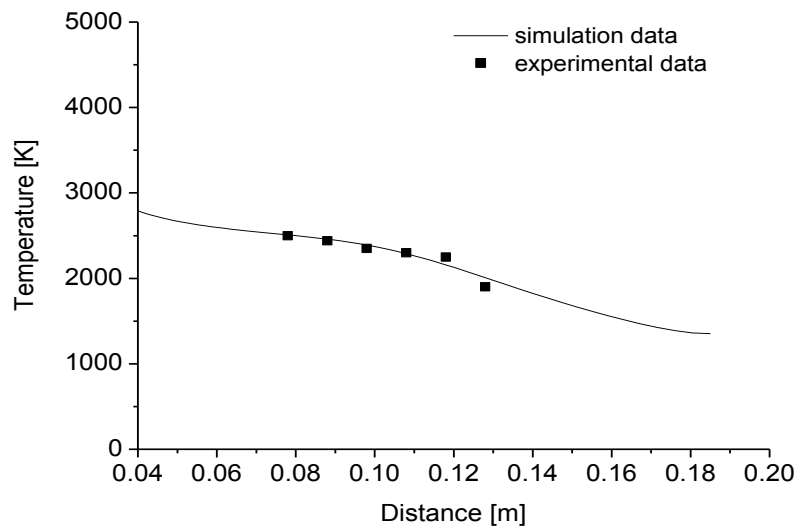
Figure8 : Computational domain

Figure9 : Comparison of computed and experimental axial values of temperature for 0.1 SLPM
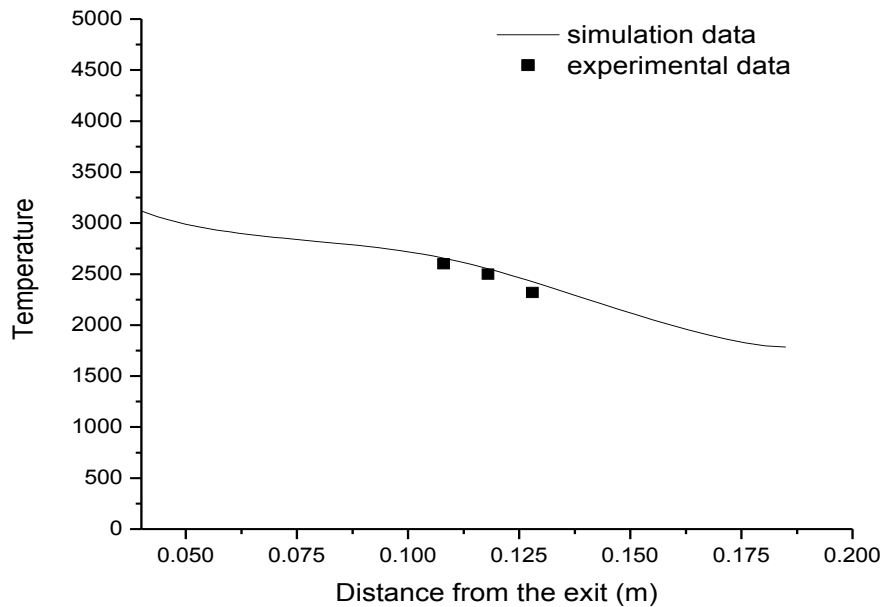
Figure 10 : Comparison of computed and experimental axial values of temperature for 0.14 SLPM

5. OBSERVATIONS AND RESULTS

Fig. 11 shows the axial temperature profile of LPG and BMCG flame as measured by the line reversal method.
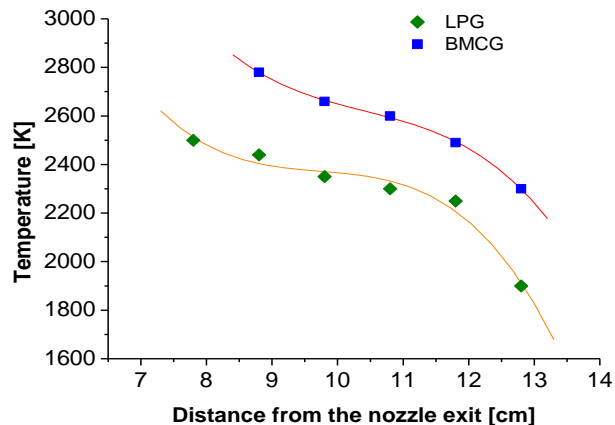

Fig.11: Axial temperature profile of flame by LPG and BMCG at fuel flow rate of 0.1 SLM and Oxygen just above stoichiometry (Just Oxidizing flame).

Flame temperatures measured at different axial locations for LPG and BMCG are recorded in Table 1. The primary flame temperature measured very near to nozzle for LPG and BMCG at the same fuel flow rates were measured by spectroscopic method. Temperature measured by line reversal method at different distances from the nozzle is also given in the table. It was observed that when the fuel flow rate increased, it was not possible to measure flame temperature close to the nozzle by line reversal method as the temperature was higher than 2800 K. Fig. 12(a) shows the axial temperature profile for secondary flame by line reversal technique and the primary flame temperature measured by the spectroscopic technique. It is observed that the region between primary flame and the point at which the flame temperature drops below 2800 K is at higher temperature for both, the BMCG and LPG. Primary flame temperature is slightly higher for BMCG as compared to that for LPG.   In the secondary flame, it is clearly observed that the BMCG flame temperature is about 250 to 350 ^{0}C higher than the LPG flame temperature under similar volume flow rate of fuel and oxygen supply just at or slightly above stoichiometry. In Fig. 12(b) when

the fuel flow rate is increased to 0.14 SLM, Only two readings for BMCG within the scanning range of our X-Y-Z table could be obtained, indicating that the secondary flame temperature is higher at distances closer than 12 cm from the nozzle of the torch. In this case too, the primary flame temperature for BMCG as measured by the spectroscopic technique is higher than that of LPG. Fig. 12(c) shows the same graph for fuel flow rate of 0.18 SLM. Only one reading for LPG could be obtained by line reversal as the flame length is high. Difference in primary flames of LPG and BMCG is only about 50 to 120 ^{0}C for all the fuel flow rates.

Table-I

Flame temperature for different distances from the nozzle

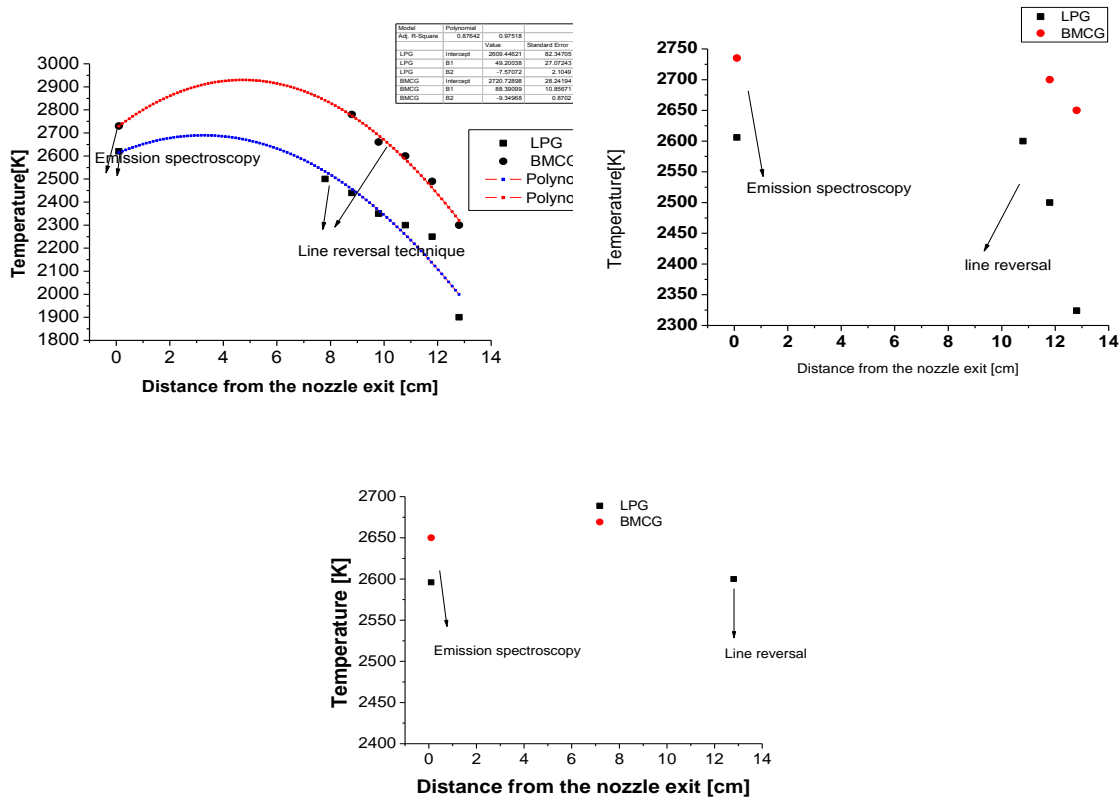| Distance from the nozzle exit [cm]	LPG At 0.1SLM	BMCG At 0.1SLM	LPG At 0.14SLM	BMCG At 0.14SLM	LPG At 0.18SLM	BMCG At 0.18SLM
0.1	2620	2730	2606	2735	2596	2650
7.8	2500		--	--		
8.8	2440	2780	--	--		
9.8	2350	2660	--	--		
10.8	2300	2600	2600	--		
11.8	2250	2490	2500	2700		
12.8	1900	2300	2324	2650	2600	

Fig. 12: Temperature profile for LPG and BMCG flames at fuel flow rate of a) 0.1 SLM b) 0.14 SLM c) 0.18 SLM

Figure 13 shows the photographs of the flames produced by LPG and BMCG for fuel flow rates 0.1SLM with Sodium seeding and without Sodium Seeding[7].
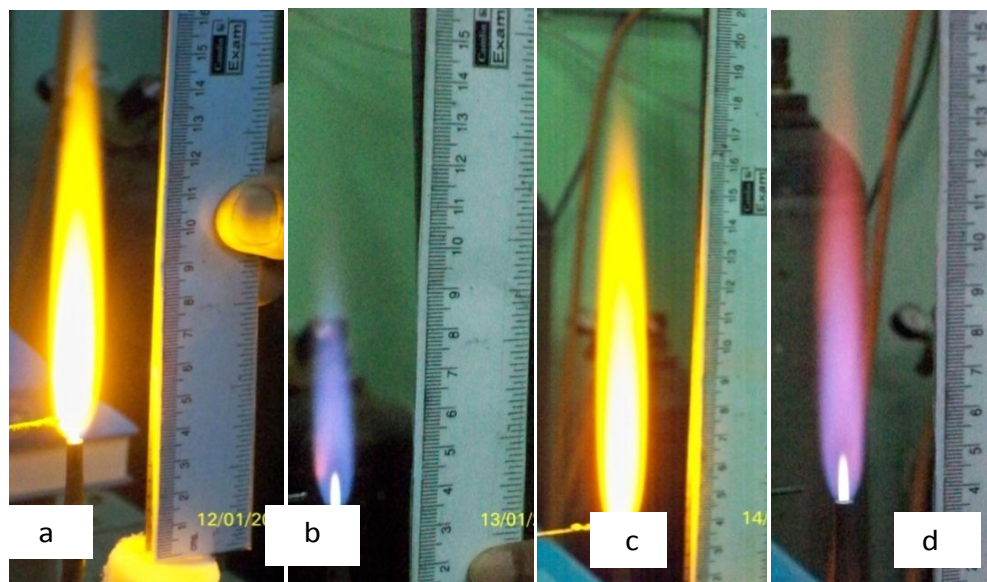
Fig. 13: Photographs of the flames with BMCG and LPG at flow rate 0.1 SLM a)LPG with sodium seeding b) LPG without sodium seeding c)BMCG with sodium seeding d) BMCG without sodium seeding

5. CONCLUSION

Sodium line reversal method was used to measure temperature in secondary flame region and Boltzmann plot method was used to measure temperature in bright primary flame, near to the torch nozzle. The primary flame temperature measured by Spectroscopy for BMCG is higher by about 50 to 120^0C than that for LPG. The secondary flame temperature measured beyond about 8 cm from the nozzle is higher by about 250 to 350 ^{0}C than that of LPG under same fuel flow rate. Highest temperature zone of the flame lies in the secondary flame and is closer to the primary flame. Accuracy of measurement is +/- 20^0C for the line reversal method and its range is from about 1600^0 C to 2800^0C. For spectroscopic measurements the accuracy is about 3%. Spectroscopic & line reversal methods have been applied to flame temperature measurements of high energy fuels i.e. LPG and BMCG. A CFD simulation matched with the experimental data points.

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