Determination of Gas Liquefied Petroleum Flame Temperatures Using Emission Spectroscopy

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Abstract

Emission spectroscopy was used in the temperature determination of LPG (Liquefied Petroleum Gas)pre-mixed flames. Natural emission of from CH* radicals was investigated in premixed flames under three different burning conditions: fuel/oxydizer stoichiometric ratio, fuel excess (rich flame), and oxydizer excess (lean flame). CH* rotational temperature of 2845 ± 70 K were measured with the setup used in the experiments. This value did not show significant change with respect to the type of flame analyzed and it is compatible with the calculated adiabatic flame temperatures of the investigated systems, which varied from 2857 K (rich flame) to 2910 K (lean flame). Temperature results obtained from this radical spectra emission are also comparable with the flame translational temperature. This temperature value agrees with that determined by an indirect measurement, using the sodium line-reversal method. This technique was chosen because the emission measured is absolutely independent from the flame natural emission and its use is well established in literature.

Introduction

Flame temperature determinations provide an important information about the heat released in chemical reactions that occurr in combustion systems [1]. The knowledge of the temperature distribution in a combustion chamber can indicate eventual project problems can give data used in construction optimization of these devices [2]. Temperature diagnostics usually is carried out by thermocouples and suction pyrometers. Both techniques are intrusive, because these devices are inserted into the flames, changing their characteristics.

The emission of radiation from the flame hot gases have an absolutely non-intrusive characteristic and offers several possibilities of temperature monitoring and equilibrium studies of flames [3,4]. Moreover, it is a very simple method, compared to the other laser spectroscopic techniques [5-8].

Spontaneous (or natural) emission in flames is due to chemical reactions that produce chemical species in the excited state. This phenomenon is also known as chemiluminescence. Among the several species found in hydrocarbon flames, the radical CH* has been used in flame mapping, due to its intense emission bands in the ultraviolet-visible region [9]. The most intense system is observed around 431.5 nm, that corresponds to the $(A^2\Delta - X^2\Pi)$ transition [10].

The lack of thermal equilibrium in a flame does not permit the use of the classical temperature concept, as measurement of the total kinetic energy [11]. However, in flames, the rotational temperature is very close to the kinetics temperature, due to the quick transfer rate between the rotational and translation energies [12]. In this work, we have used the ro-vibronic emission spectra of CH* radicals to determine the temperature of Liquefied Petroleum Gas (LPG) flames.

Experimental Setup

Flames were produced from a gaseous mixture of LPG/atmospheric air/oxygen. Oxygen employed to obtain flames with different equivalence ratio (ϕ) (Table 1). LPG was considered as a propane/n-butane equimolar mixture. The burner fuel and oxidizer supply was controlled by calibrated flow meters.

The optical system used was a TRIAX 550 (Jobin Yvon) monochomator with 0.5 m focal length (f), equipped with a 1200 lines.mm⁻¹ diffraction grating, with blaze at 500 nm and slit width of 10 μ m. The emission signal was detected by a Hamamatsu R928P phototube. Spectra were obtained in the 415 to 440 nm range, which corresponds to the A² Δ -X² Π CH^{*} electronic band.

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Flame (ϕ)	Total O_2 (mmol.min ⁻¹)	$N_2 \text{ (mmol.min}^{-1})$	LPG (mmol.min ⁻¹)
Rich (1,43)	21,2	27,9	6,3
Stoichiometric (1,02)	35,5	27,9	6,3
Lean (0,78)	46,8	27,9	6,3

Table 1- Burner conditions used in the chemiluminescence measurements

The burner was mounted on a base with mobility in the three orthogonal directions. A quartz lens (f = 100 mm, diameter = 2") was used for light collection. The flame image was projected in the spectrometer entrance slit at a 1:1 ratio. The apparatus scheme is shown in Figure 1.



Figure 1: Experimental apparatus.

Flame temperature was determined using the Boltzmann plot method [13]. This technique is based on the measurement of the band intensity of a chemical species, in this case, the radical CH^* . The relation between the line experimental intensity (*I*) and the temperature (*T*) for a specific transition is given by the Equation 1:

$$I = CS_{J'J''}\lambda^{-4} \exp(\frac{-E_{J'}}{kT}) \qquad \text{Equation 1}$$

where $S_{JJ'}$ 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 proportionally constant. If the system shows a 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.

Flame temperatures were also determined by the sodium reversal line method [14]. This is a simple and well established method, which has been largely used is the last decades. The comparison between emission intensity of a seeded species in the flame, usually sodium atoms, with the radiation emitted by a black body is the basis of the procedure for the measurements.

Results and Discussions

No remarkable differences in emission spectra features were observed in the investigated flames. A stoichiometric flame spectrum, obtained at a 2.5 mm height, is shown in Figure 2.

CH* emission spectra show an intensity maximum, as predicted, 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 formed predominantly by the R-branch of the 0-0 band, with J value from 11 to 20. For $J \ge 7$ this branch shows a rotational structure sufficiently spaced with no interference from other peaks and adequate for intensity measurements. This region, which appears as doublet peaks, was used for rotational temperature determination by simulation and application of the Boltzmann's method.





Figure 3 corresponds to a typical Boltzmann's plot obtained from an average of three experimental spectra from stoichiometric flames, at 2.5 mm. Each point in the graph, therefore, corresponds to the measured intensity and the traced line is a linear regression calculated, from whose slope was used for the determination of the rotational temperature.



Figure 3: Boltzmann's plot for CH^{*} stoichiometric flame spectra. Temperature = 2830 ± 47 K.

The linear shape shown by the plot at Figure 3 indicates that the radical CH* population of rotational energy states presents a Boltzmann's distribution. Similar plots have been constructed for other spectra obtained. These results are shown in Table 2 and Figure 4.

Rotational temperatures did not present an appreciable variation with respect to equivalence ratio and distance above the burner. The temperature distribution suggests an adiabatic behavior of the investigated flame region, which corresponds to the central part of the flame reaction zone, i.e., the inner cone, where chemiluminescent process are most intense. Indeed, rotational temperatures are very close to the flame adiabatic temperature: 2857 K, 2946 K and 2910 K for rich, stoichiometric and lean flames respectively, in comparison with an average experimental value of 2845 ± 70 K.

To confirm this hypothesis, flame temperature was determined by sodium line-reversal spectroscopy. Average value obtained by this technique, 2930 \pm 88 K, is very close to the results observed by emission spectroscopy.



Distance (mm)	T (K)		
	$\phi = 1.43$	$\phi = 1.02$	$\phi = 0.78$
5.5	2793 ± 71		
4.5	2965 ± 66		
3.5	2878 ± 125	2783 ± 26	2872 ± 76
2.5	2784 ± 60	2859 ± 47	2817 ± 58
1.5	2752 ± 129	2895 ± 37	2900 ± 71

Table 2- temperatures for CH* as a function of equivalence ratio (ϕ) and burner distance (mm).



Figure 4: Temperatures for CH^{*} as a function of the equivalence ratio (ϕ) and burner distance (mm)...

Conclusions

CH* emission spectroscopy has shown to be an adequate technique for flame temperature determination. Variation of the rotational temperature as not observed when the flame composition changed for the investigated flames. The determined average temperature was 2845 ± 70 K. This value is close to the flame adiabatic temperatures: 2857 K, 2946 K and 2910 K, which corresponds to rich, stoichiometric an lean flames respectively. Measurements of rotational temperatures were found to be in good agreement with the sodium line-reversal results.

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