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EMISSION SPECTROSCOPY OF CH RADICAL TO DETERMINE THE TEMPERATURE OF ETHANOL FLAME*

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Abstract

The aim of this work is to avaluate the temperature of an ethanol/air mixture in a diffusive flame by analyzing the emission spectra band of CH radical, through comparison with simulated spectra obtained by the LIFBASE software. The temperature in the blue zone of the flame was 2300 K. These results agree with the calculated temperature based on the GASEC software, witch use thermodynamic data.*

Introduction

The light emitted by the flame may be used to monitor and control combustion[1]. Several phenomena contribute to the light emission process. Discrete emission spectra in the UV-visible range (chemiluminescence) correspond to electronically excited species produced in the chemical reactions in the flame:

$$A + B \rightarrow C + D^*$$

This chemically excited radicals or molecule D* may be destroyed by spontaneous emission ($D^* \rightarrow D + h\nu$) or collisional quenching ($D^* + M \rightarrow D + M$). Chemiluminescence corresponds to the spontaneous emission of photons ($h\nu = E_2 - E_1$ with E_2 the energy of the excited state and E_1 the energy of the fianl state). This emission generally takes place in the UV or visible range. Each molecule or radical produced in an excited state is responsible for a particular spectrum, witch is related to its quantum properties, and can be identified.

The radiative decay of excited species as the (0,0) band transitions of OH ($A^2\Sigma \rightarrow X^2\Pi$), CHO ($A^2\Pi \rightarrow X^2A'$), CH ($A^2\Delta \rightarrow X^2\Pi$) and C_2 ($A^3\Pi \rightarrow X^3\Pi$) are mainly responsable for the chemiluminescence observed in the combustion of hydrocarbon fuels [2], however, the chemical processes of excited species formation has not yet been definitely established. Very little attention has been directed in recent studies to the formation of excited species [3 – 9].

In this work, the spectra of the natural chemiluminescence's CH* radical in ethanol/air flame was detected and compared with that simulated with LIFBASE software to estimate the temperature.

Experimental Setup

Figure 1 illustrates the experimental setup. The system includes a homemade burner to be used with liquid fuel, a lens with 50 mm focal lenght, a ½ m monochromator with slit width of 0.1mm, resulting a spectral resolution of 0.2 nm, coulpled to a photomultiplier. The signal of the photo multiplier was registered in a single XY recorder and the data was worked with Math Cad software to transform to digital the analog data. The burner inject include a system to inject at the same time the alcohol and air (alcohol atomizer), and the flow rates were measured with a rotameter. The burner and the quartz lens were put in XYZ translator so the flame and the lens can be moved to obtain the best emission signal detected by the photo multiplier. The standard experimental conditions were: 2.5 mL/min of ethanol and 1100 mL/min of air. This air is used to atomize and vaporize the ethanol and also in the combustion process.

Figure 2 shows a photo of the ethanol flame obtained in the above conditions.

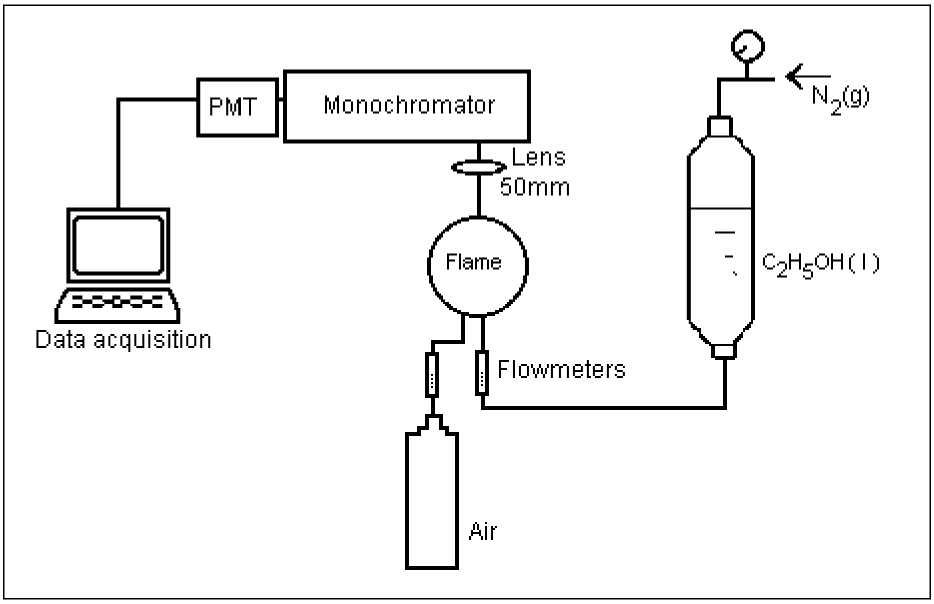

Figure 1: Schematic of the experimental setup

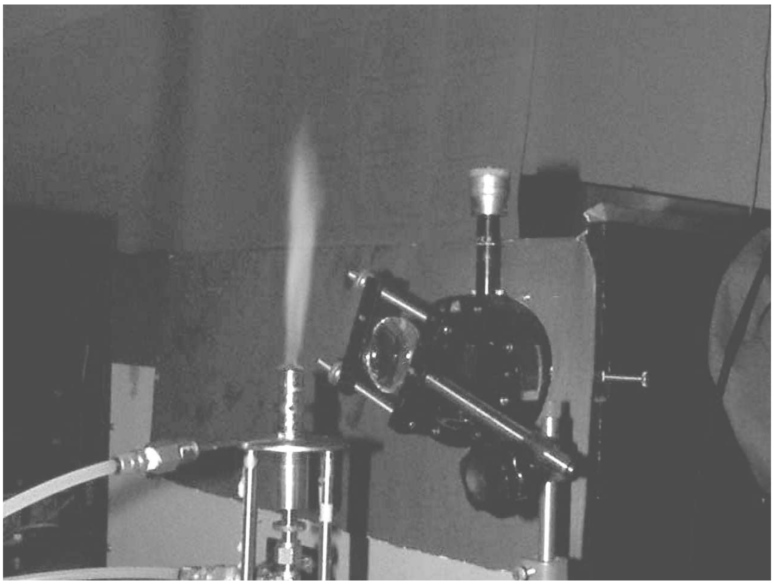

Figure 2: Photo of burner used in the experiment.

Results and Discussions

Figure 3 shows the emission spectra of the CH radical from 425,5 to 440 nm obtained experimentally and the simulated spectrum calculated by the LIFBASE program. As can be observed, the intensity of the peaks in the region from 425,5 to 433,5 nm are much stronger compared to the 433,5 to 440 nm range, where the peaks are small and not very well defined experimentally. Therefore, we chose the 425,5 to 435,5 nm range to evaluate the temperature. Figure 4 shows both the experimental (continuous line) and the simulated (LIFBASE calculated, dotted line) spectra for a temperature of 2300 K. The spectra agree reasonably. Absorption spectroscopy measurements with diode lasers in a oven [10] showed a temperature of 1500 K. Below are some temperature calculations for the combustion of ethanol in air using the GASEC software:

Mixture composition	Temperature
Stoichiometric combustion	2347 K
10% lean in ethanol	2230 K
10 % excess ethanol	2304 K
20 % excess ethanol	2263 K
30 % excess ethanol	1976 K

It seems clear that the difference between the temperatures measured by emission spectroscopy and by diode laser absorption spectroscopy is due to the different positions of the flame that were measured, to the different conditions of the combustion and because in the laser absorption method a mean temperature is obtained, related to the optical pathway of the laser radiation through the flame, while the emission seen by the detector comes from an almost punctual source. All measurements reported here were made in the blue region of the flame, near the exit of the burner. It must also be pointed out that the combustion of the alcohol uses predominantly the atmospheric oxygen: in the burner, the ratio air/ethanol corresponds approximately to a 12 times lower ratio than the stoichiometric quantity. (for an ethanol flow rate of 2.5 mL/min corresponds an air flow rate of 13672 mL/min for a stoichiometric burning, while the atomization air flow rate was only 1100 mL/min, approximately)

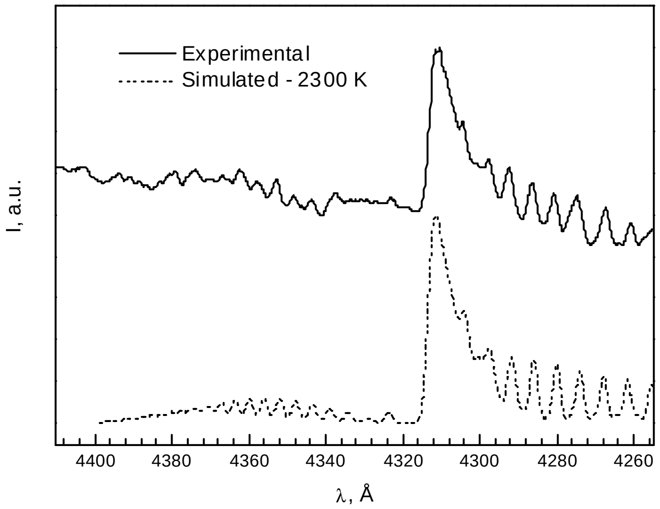

Figure 3 Theoretical and experimental spectra in the 4400 Å and 4260 Å range

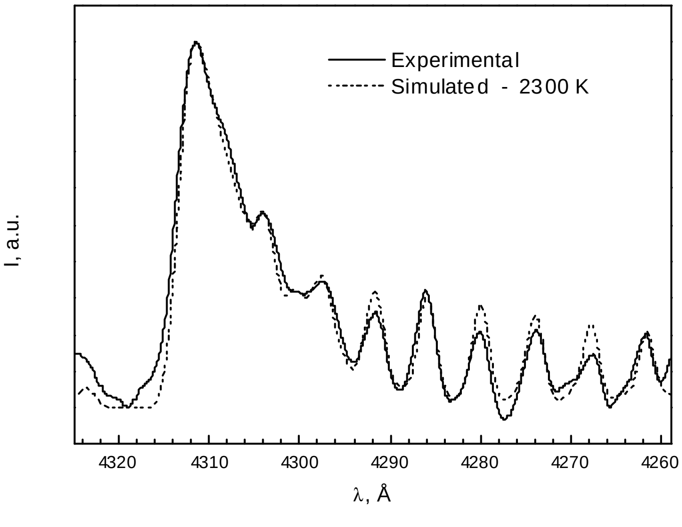

Figure 4: Experimental and theoretical spectrum.

Conclusions

The temperature obtained through the emission spectra of the blue zone of an ethanol flame by comparison with LIFBASE simulated spectra was 2300 K. This results agrees with the temperature calculated through GASEC software. that uses thermodynamics data for the system. The use of emission spectra of the CH radical to estimate the temperature of the flame the combustion of ethanol seem to give results close to thermodynamic calculations.

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