

Experimental Characterization of a Laboratory Flame through “Time-Resolved High-Resolution Optical Emission Spectroscopy”

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Abstract During the combustion, such as the one occurring in the combustion chambers of rocket engines, the maximum temperature is reached in the combustion zone. Knowing the position and the temperature of this zone is of fundamental importance to optimize both the efficiency of the combustion engines and their design.

Optical Emission Spectroscopy (OES) is a good alternative to any intrusive technique to achieve the above-mentioned goals without disturbance in the analyzed flow, by detecting the chemical markers of combustion zone such as the *CH* and *C₂* radicals. The work presented in this paper was performed at the Propulsion Laboratory of CIRA, in the framework of the HYPROB program.

Time-resolved High-resolution OES was used in the position and temperature determination of the combustion zone of a laboratory butane flame. This technique was applied using an innovative experimental apparatus that allows the investigation of the combustion process with a high spatial and temporal resolution. In particular, several spectra were acquired simultaneously along the axial direction of the flame propagation by a bundle of optical fibers, both for premixed and diffused flames. These spectra have provided the position of the combustion zone and its temperature, by the analysis of spontaneous radiation emitted by the *CH* and *C₂* flame radicals.

Keywords: Chemiluminescence, Butane Flame, *CH* and *C₂* radicals, Optical, Combustion Diagnostics

1 Introduction

Today's principal interest in combustion processes is about their optimization. This goal can be reached through a deep knowledge of the chemical processes, products of chemical reactions and their quantity [1] [2] [3].

Combustion is a high-temperature exothermic redox chemical reaction which involves oxidation of *fuel* by the *oxidant* that usually produces lot of heat, light and also chemical products like *CO₂*, *CO* and *H₂O*. In most chemical reactions oxidant is atmospheric oxygen but in other cases it could be something different.

The chemical components get the maximum temperature in the combustion zone of the flame. This zone divides which is burned from which is not burned yet. Knowing its position and its temperature is of fundamental importance, for example, to combustion chamber design. In fact through these information is possible to correctly size the cooling systems of surfaces. In this way it is possible to save weight during the engine design. Another advantage could be saving fuel thank to the optimization of the combustion process.

Spectroscopy is a valid alternative to intrusive techniques to manage quantitative analysis about presence of chemical species and the temperature of the combustion zone. Intrusive methods are not so reliable as non-intrusive ones to catch the presence of chemical species and their temperature because they need to get in touch with the flow under analysis generating, in that way, a flow disturbance. In addition, they are not able to undergo the high temperatures reached in the combustion zone.

Spectroscopy allows the study of electromagnetic radiation for wavelength between Ultraviolet (UV) and Near InfraRed (NIR). The products of combustion such as *H₂O*, *CO* and *CO₂* emit radiation in the IR wavelength range, but their spectra are continuous. On the other hand, the *OH*, *CH* and *C₂* radicals are formed in abundance in the combustion zone and emit well-defined bands in the range of UV-NIR wavelength. These radicals have a very short average life (about 10⁻⁶s). This involves the advantage of acquiring their emission exactly in the area under investigation.

The aim of this article is the description of both the innovative experimental apparatus designed for the application of “Time-resolved High-resolution OES” technique and the preliminary results obtained applying this system to the experimental characterization of a laboratory butane flame to identify the combustion zone and its temperature.

The article will be divided in three sections. The first will give some brief theoretical bases in order to properly approach the *OES* technique, the second will describe the experimental apparatus and the last will present preliminary results and conclusions.

2 *OES* theoretical review

Spectroscopy studies energy transitions between energy levels of a system made of atoms and molecules. When some of matter absorbs electromagnetic radiation the matter itself withstands a change in its energy content. Nowadays is commonly approved that electromagnetic radiation can be seen as particle beam. These particles are called *photons*. When a photon is absorbed by matter the driven energy is absorbed by matter and the photon itself is not traceable any more.

Energy of a photon E in Joule [J] is strictly linked to its frequency ν [1/s], to its wavelength λ [m], to its wave number $\bar{\nu}$ [1/m] and to speed of light through the matter c [m/s] by the following relationship

$$E = h\nu = \frac{hc}{\lambda} = hc\bar{\nu} \quad (1)$$

where h is the Planck constant which has a value of $6.626 \times 10^{-34} \text{J} \cdot \text{s}$.

The energy absorption by an atom (or a molecule) happens only when the photon's energy $h\nu$ is exactly the same of the energy difference ΔE between two energy levels taken into account. When a body absorbs a certain quantity of electromagnetic radiation, the number of photons which pass through the body is not the same as the incident ones, but it is less. A measure of this decrease is called *absorbance* (or *absorptivity* in opposition to *emissivity*). When, instead, an atom (or a molecule), which is in an excited state, returns to a lower energy state, the energy excess is released, once again in form of photons, through a process said *emission*. It is important to note that each energy level has a well-defined value since each state energy is quantized.

The attention will be particularly concentrated on transitions which bring to formation of excited CH and C_2 (indicated with a star where the molecule is excited). As reported in [4] studies suggest that CH^* might be formed from the following reactions:



while C_2^* could be brought from the following:



So the primary combustion zone of the analysed flame will be distinct from the other parts of the flame itself by its emission, namely CH bands at 387nm and 432nm and C_2 bands between 436nm and 563nm.

2.1 Forms of energy and energy breakdown

Taking into account the typical *dumbell* molecule made of two atoms it is possible to recognize different forms of energy:

- *translational energy* E_{trans} : it represents kinetic energy of center of mass of molecule. In this case speed can be decomposed along the three Cartesian coordinates (u , v , w) of a generic inertial coordinate system.
- *rotational energy* E_{rot} : it represents the rotational energy which causes motion of the molecule in the local coordinates system.
- *vibrational energy* E_{vib} : this energy is due to the vibrational motion of atoms around the equilibrium position.
- *electronic energy* E_{el} : this form of energy is due to the motion of electrons around the nucleus of every atom of the molecule. This energy, associated to each electron, can be split in two parts: kinetic energy of electrons during their translational motion around nucleus, and potential energy due to electron position respect to the nucleus.

So the total energy of a diatomic molecule may be seen as the sum of these contributions of energy just described. In molecular spectroscopy it is usually to talk about the *Born-Oppenheimer approximation* which is the conceptual simplification that the energy contributions are handled separately. In this way they do not interfere with each other in any way. In formulas:

$$\text{for a molecule} \rightarrow E = E_{trans} + E_{rot} + E_{vib} + E_{el} \quad (6)$$

$$\text{for an atom} \rightarrow E = E_{trans} + E_{el} \quad (7)$$

To complete this energy breakdown is necessary to take into account the so-called *energy ground level* E_0 . This energy level is a very low one and it is associated to the energy owned by a molecule at the absolute zero temperature. According to this position total energy is measured starting from the *ground level* and not from the zero value that would be a conceptual error.

$$E = E_{trans} + E_{rot} + E_{vib} + E_{el} + E_0 \quad (8)$$

It is important to note that energy shifts from ground energy to an excited state (the energy shift is denoted by ΔE and expressed in terms of wave number) are different for each form of energy. Electronic jumps are the highest ones as it is clear from the following approximations chain:

$$\Delta E_{el} \approx 10^3 \cdot \Delta E_{vib} \approx 10^6 \cdot \Delta E_{rot} \quad (9)$$

Within each electronic energy level it is possible to find electronic vibrational sub-levels and, in the same way, within each vibrational energy level it is possible to find rotational sub-levels.

At this point it is necessary to introduce the concept of *population of an energy level*. Population of an energy level is one of those factors that influence and determine the intensity of the spectral lines. The population indicates the number of molecules that can be found in a given energy state. Assumed good Boltzmann model, for a sample of gas at absolute temperature T and having a number of molecules N , the number of molecules having energy E_j is given by the Boltzmann statistic distribution. So if we have N_0 molecules in the lowest state, N_j molecules in a higher state J , ratio between these population is given by:

$$\frac{N_j}{N_0} = e^{(-E_j/kT)} \quad (10)$$

where E_j is the energy at excited state and k is the Boltzmann constant. It is possible to generalize the equation 10 taking into account the shift between two energy levels, both different from the ground level, with an energy difference of ΔE . It is valid the following relationship:

$$\frac{N_j}{N_i} = e^{(-\Delta E/kT)} \quad (11)$$

where N_j is the number of molecules that occupy the higher energy level and N_i is the number of molecules that occupy the lower energy level.

From equation 11 it can be noticed that an increasing temperature T causes an increasing in the number of particles which experience the excited state. In the same way, an increasing energy shift ΔE means a decreasing number of particles which experience the excited state. In this way a different temperature causes a different population in each energy level. This is the main reason of changes in spectra. Thanks only to the shape of spectra it is possible to identify which and at which temperature transitions happen.

3 Experimental apparatus

The main components of the experimental apparatus are: a bundle of ten optical fibers, a monochromator and an intensified CCD.

The radiation emitted by the analysed flame is brought through the optical fibers to reach the monochromator *entrance slit*. The ten optical fibers allow to acquire radiation emitted by the flame in ten different zones.

By the use of collimators (OZ-Optics), properly interfaced to the optical fibers, various flame zones are focused and the beams of electromagnetic radiation are made parallel to each other. The link between optical fiber and monochromator is made by a cylindrical interface called *bundle* which keeps separated radiation coming from each of the ten fibers.

The monochromator (Acton SP 2500) has a focal length 0.5m and a set of three gratings, with 150, 1200 and 1800 *grooves/mm* and blaze at 500nm. Each grating separates the incident polychromatic electromagnetic radiation into its monochromatic components. The monochromatic signals are then sent to the intensified CCD (PI-MAX: 1024i) which increases intensity of signal and then digitizes it. The intensified CCD has resolution of 1024×1024 pixels, maximum gain 60 and minimum exposure time of picosecond.

In Figure 1 is shown a schematic representation of the instrumentation used in this work.

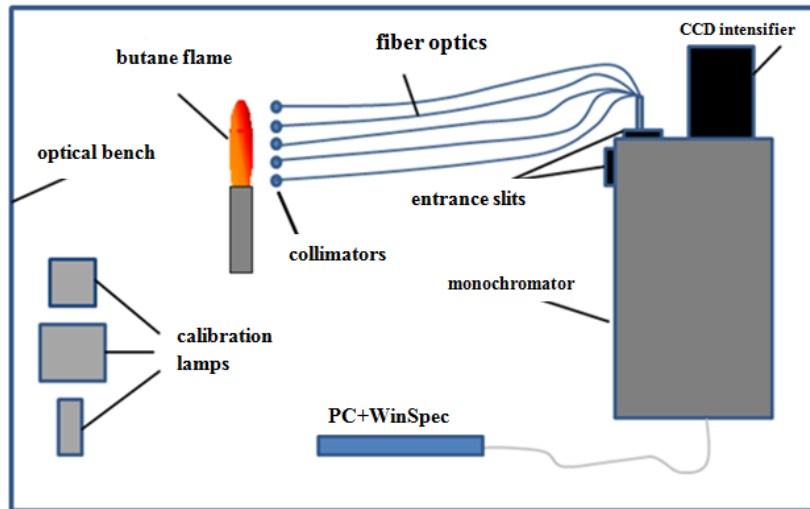


Fig. 1 Schematic representation of experimental apparatus.

The whole apparatus is placed on an optical bench to have a perfect horizontality of each optical fiber and to isolate all optical components from random vibrations.

The system is controlled by the software Synergy, that allows the acquisition of spectra by setting time exposure, wavelength range and acquisition rate. More details on the instrumentation are given in the following sections.

4 The main components of measurement chain

In this section we will briefly describe the main components and their technical specifications.

4.1 Monochromator Acton SP 2500

The monochromator is equipped with a slot (also called *entrance slit*) which is the entrance to the device for the emitted radiation. The slit is made of two knives which manage the quantity of light that has to enter in the monochromator. Thanks to a very fine pitch screw it is possible to adjust the width of the slit up to an hundredth of millimetre. Reduction of the gap between knives of slit involves an increase of spectral resolution.

In figure 2 we can see the full path of a polychromatic beam of light in a typical monochromator: from entrance slit to the intensified CCD camera. The emitted radiation by the source starts as polychromatic radiation from the point A and passes through the entrance slit (located at point B in figure 2). After that, light reaches a mirror which works as collimator (it makes parallel each ray constituting the white light beam). The single rays are then redirected to a diffraction grating placed in D. Each beam of white light is separated into its single monochromatic components. The monochromatic rays then proceed towards a second mirror (placed in E) which has the job of focusing the light. The monochromatic rays are then redirected by this mirror to the exit slit of the monochromator (placed in F). The G spot is the camera that acquire the radiation emitted by the

analysed source in a certain wavelength range. The acquired radiation is represented by the green light beam in the figure.

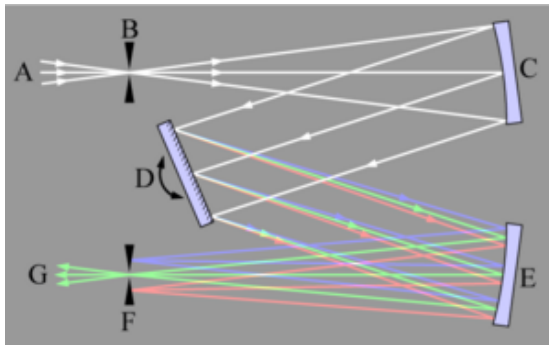


Fig. 2 Typical path made by a beam light in a monochromator.

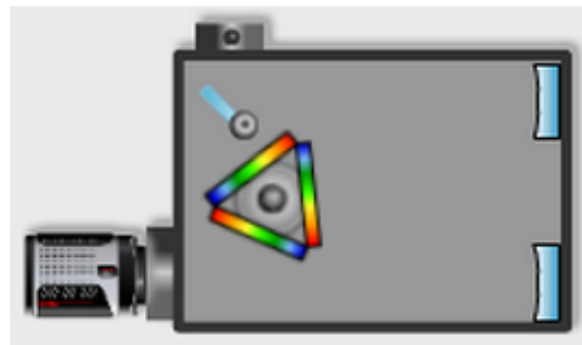


Fig. 3 Schematic representation of *Acton SP 2500* monochromator used for experimental proofs.

The main characteristics of *ACTON SP 2500* monochromator are the following ones.

1. The *ACTON SP 2500* monochromator is internally equipped with a turret on which are built three gratings, each with a different groove density. The three gratings have respectively 150, 1200 and 1800 *grooves/mm*. Briefly, a bigger groove density lets see the fine structure of particular emitting radicals. On the other hand, because of the fact the same amount of energy has to be divided among all grooves a greater number of grooves causes a less bright spectra.
2. The *sensible range* of monochromator goes from 0nm to 1400nm. This is the wavelength range in which the gratings of monochromator are theoretically able to acquire some radiation.
3. The last main characteristic it is useful to report about the monochromator is the focal length of 500mm. Increasing the focal length allows to spread more largely the monochromatic light beams.

4.2 Intensified CCD camera PI-MAX4:1024i

The intensified CCD camera *PI-MAX4:1024i* allows to scan multi-point high frequency time-dependent spectra with a large pixel resolution. The fiber bundle is the component which allows to run experiments with ten different points of observation along the flame extension.

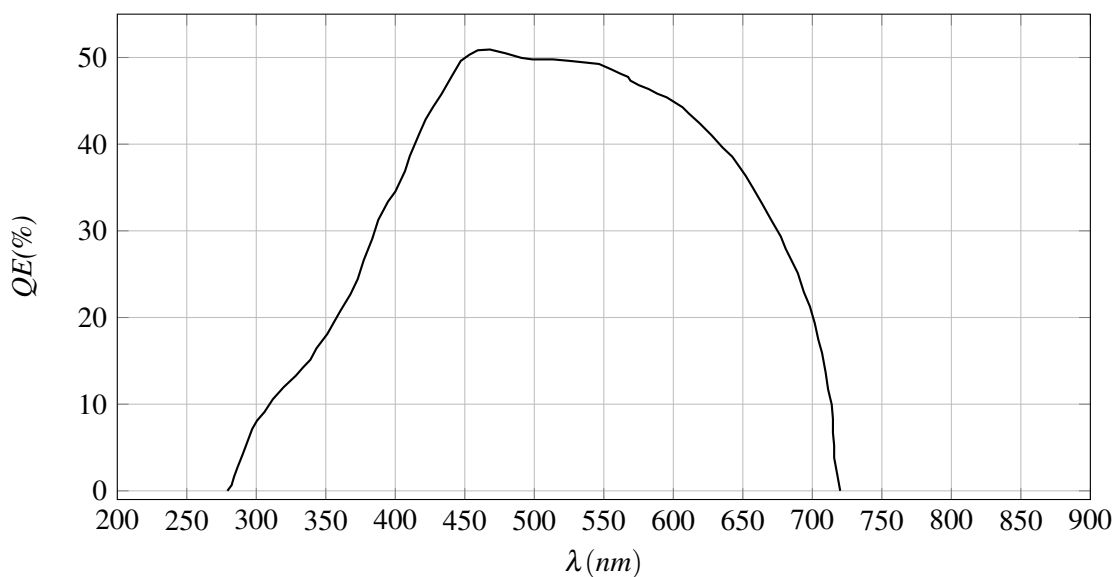


Fig. 4 Variation of quantum efficiency with wavelength of *PI-MAX4:1024i* camera sensor.

The *PI-MAX4:1024i* camera, produced by Princeton Instruments, records monochromatic light beams exiting from monochromator. The measurement system is characterized by a CCD sensor of 1024×1024 pixel coupled with an intensifier (from which the name of ICCD). The big number of pixels allows high resolution spectra acquisition. In addition, the intensifier makes possible to acquire time-dependent spectra varying the opening time of the gate up to values near to picoseconds. Decreasing the gate time allows to acquire spectra with a very high frequency but, of course, with a decreasing spectra maximum intensity.

In order to acquire spectra with a good signal-to-noise ratio it is useful to study radiations emitting in the most efficient wavelength range of the chosen CCD sensor. The CCD sensor efficiency is ruled by intensifier *quantum efficiency* (represented by *QE* in figure 4). In general, this is the ability of a device to convert energy (so light too) in other forms, for example in an electrical signal. The intensifier quantum efficiency curve is represented in figure 4. As we can see the efficiency reaches its maximum value at about 500nm. In general it is considered acceptable a quantum efficiency greater than 20% so it is possible to consider as acceptable wavelength range the wavelengths between 350nm and 700nm.

5 Technical approach to the experiment

The experiment has been driven with the aim of identifying the combustion zone and the temperature of the flame itself. Both these information will be caught from the radicals emission spectra shape.

Each experiment has been driven with a specific series of preliminary procedures in order to make it as much as possible repeatable.

1. The first phase is the optical set-up tuning. This means to align the slit of bundle with the entrance monochromator slit.
2. It is then of fundamental importance to calibrate the whole set-up in both intensity and wavelength. The calibration in intensity lets calculate the whole set-up efficiency curve, the calibration in wavelength is instead useful to align experimental spectrum to theoretical one.
3. The acquisition phase: it consists in acquiring spectra of analysed flame with particular sets of parameters. In this paper will be presented a series of measurements which can be summarized as follows:
 - acquisition of spectra by means of a single optical fiber varying the grating, time of exposure and gain of the camera sensor;
 - acquisition of spectra with two optical fibers simultaneously distributed along the axial direction of the flame using the best parameters of measurement set-up;
 - acquisition of spectra for premixed and diffusive flame conditions with a single optical fiber;
 - acquisition of spectra with a single optical fiber into the combustion zone with a fixed acquisition frequency.
4. As last phase there is the post-processing phase. In this phase experimental spectra are analysed to identify radicals which emit in the combustion zone, locate the combustion zone and calculate flame temperature. This last goal has been accomplished thanks to two different softwares: *LifBase* and *SpecAir*. The first has been used to analysed spectra in the range of wavelength from 300nm to 400nm while the second to analyse spectra in the range of wavelength between 400nm and 600nm.

6 Results and conclusions

In this section will be presented all most significant preliminary results about identification of radicals involved in the combustion zone and the data post-processing to determine flame temperature.

6.1 Measurements with one optical fiber on premixed flame

The first measurements have been acquired on the premixed flame with a single optical fiber in order to identify the best conditions of measurement. In particular, spectra have been acquired varying grating, exposure time and gain. The focusing region of collimator is at about 1cm along the axial extension of flame by the start of burner. All spectra have been corrected subtracting the corresponding background in order to balance the

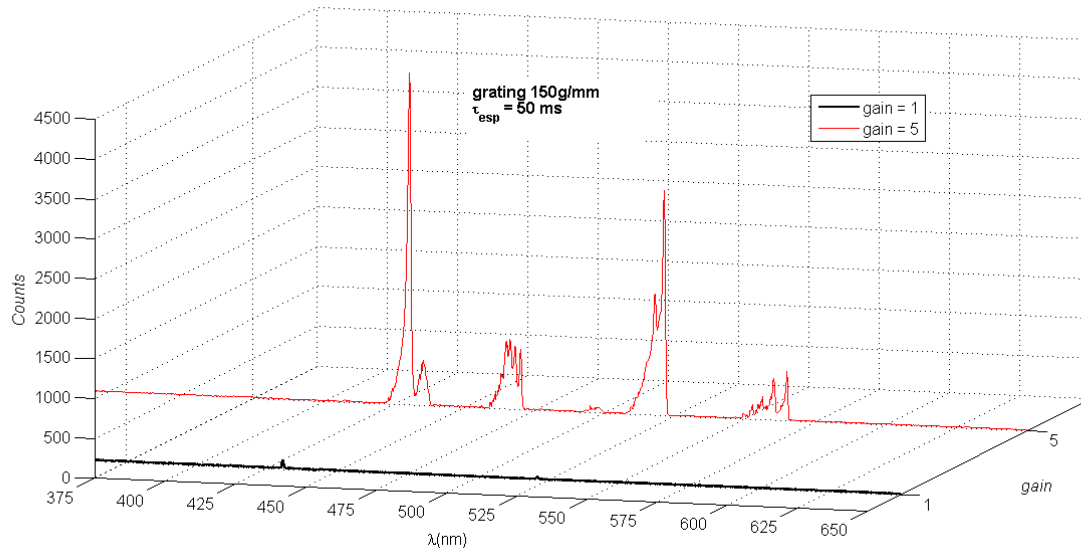


Fig. 5 Spectra of premixed flame varying the gain, exposure time 50ms and 150 g/mm grating.

contributes due to the environment noise. This is a very important operation, in fact, even if measurements have been acquired in the total dark, a small amount of environment radiation is always present.

As we can notice from the figure 5 we are not able to notice any spectra if the gain is the unity. Instead, if we increase the gain to 5 the signal-to-noise ratio is acceptable and the molecular bands are clearly visible in the acquired spectra.

Then the experimental spectra have been compared with the theoretical ones generated by the software *Lif-Base* and *SpecAir* and it has been resulted that CH and C_2 are the main responsible of emitting electromagnetic radiation in the combustion zone. In particular it is possible to attribute the bands between 432nm and 436nm to CH radical and the bands between 436nm and 565nm to radical C_2 (called Swan bands of C_2) [4].

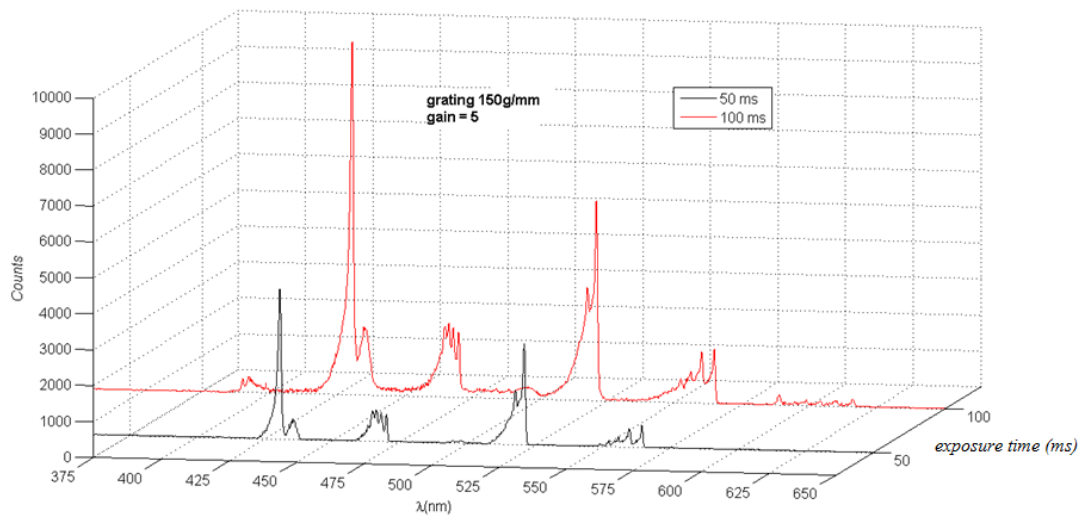


Fig. 6 Spectra of premixed flame varying the exposure time, gain 5 and 150 g/mm grating.

Because of the fact we have obtained good results with gain equal to 5 (emission bands are characterized by acceptable signal-to-noise ratio) other measurements have been acquired with this value fixed.

Figure 6 shows the calibrated spectrum of the flame obtained with grating 150 g/mm and gain 5, varying the exposure time. Exposure times are in this case equal to 50 and 100ms. Spectra show a visible improvement of signal-to-noise ratio when increasing the exposure time. This can be easily understood thinking that increasing

the exposure time means increasing the amount of radiation which get the CCD sensor. For these reasons following measures have been acquired setting the exposure time to 100ms. In particular, in figure 7 it is shown a comparison between spectra obtained varying the grating, fixing exposure time at 100ms and gain 5. It is clear

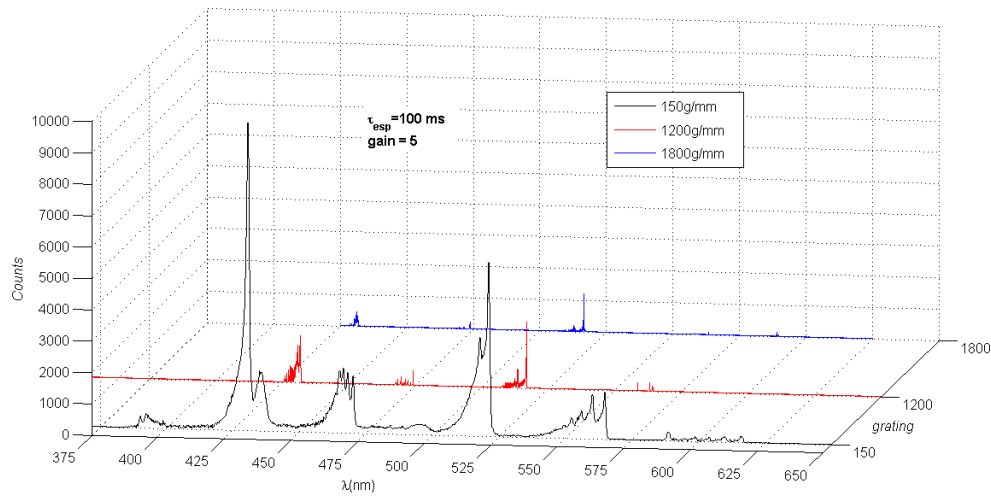


Fig. 7 Spectra of premixed flame varying the grating, exposure time 100ms and gain 5 grating.

that changing the grating increasing grooves density that decreases the signal-to-noise ratio. This is caused by the minor amount of radiation which reach each groove. However, increasing density grooves means also increasing spectral resolution. In fact, increasing the exposure time for a grating with a great number grooves allows to see the roto-vibrational structure of spectrum (Figure 8).

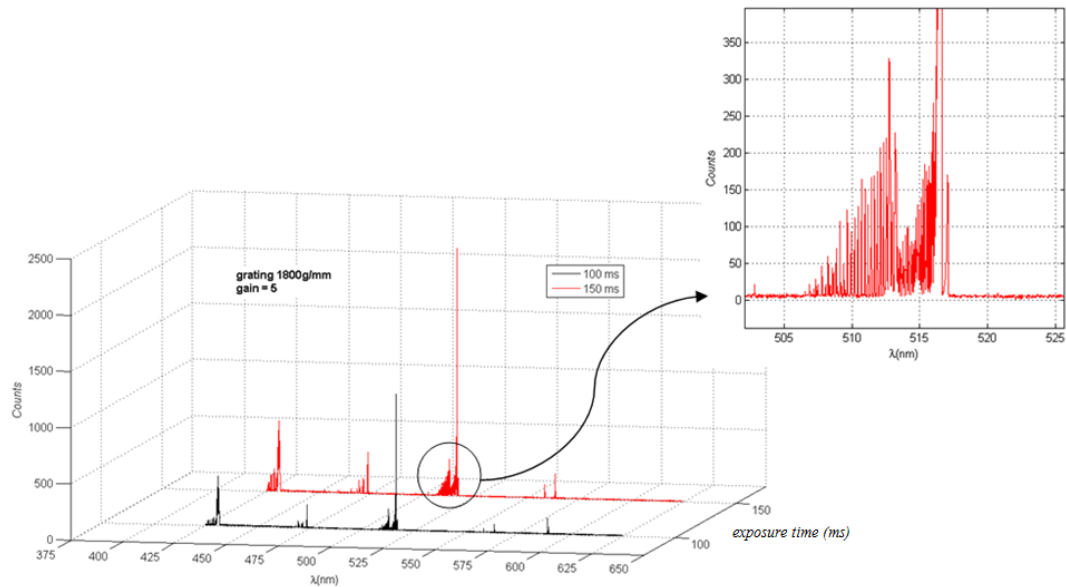


Fig. 8 Spectra of premixed flame varying the exposure time, grating 1800 g/mm and gain 5.

6.2 Measurements with two optical fibers on premixed flame

Once optimal parameters of measurement system has been identified our attention will be focused on the study of the flame in more than one point in order to identify the position of combustion zone. Two optical fibers have been used to display simultaneously two different points of the premixed flame along its axial extension. The set-up is shown in figures 9 and 10 with the indication of collimators focus distance (Figure 9) and the distance

between fibers and the output of burner along the axial direction of the flame (Figure 10). In single-point mode

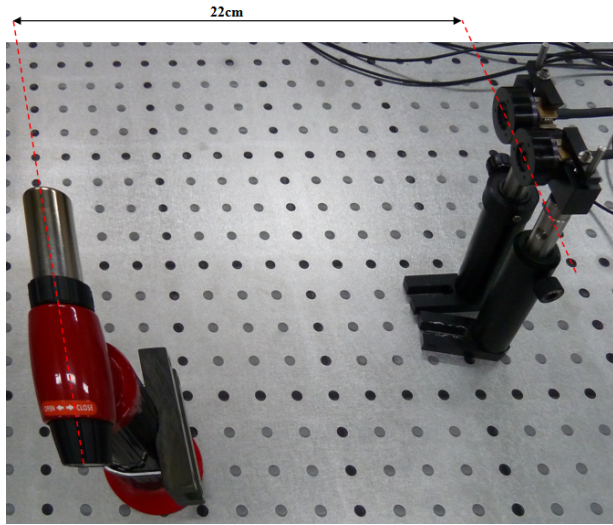


Fig. 9 Focus distance of collimators.

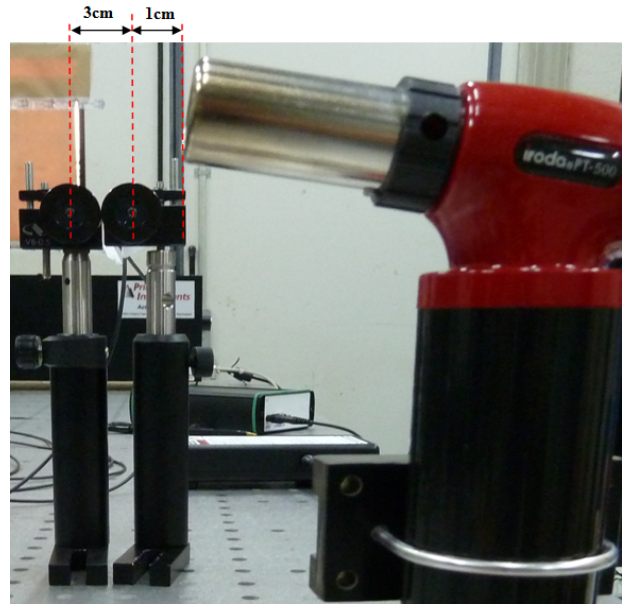


Fig. 10 Distance between fibers and burner along the flame extension.

only one fiber is active while the others are shut off. In this case two fibers are active and the acquisition software has been set on multi-point mode selecting the bundle zone to record.

The result of spectrum acquisition at 1cm and 4cm is represented in figure 11. Spectrum at 1cm from the burner exit (in the internal flame core) exhibits bands of all radicals (CH and C_2) with a very good signal-to-noise ratio. Instead, the spectrum acquired with the second fiber placed at 4cm from the burner exit shows only two bands, furthermore of low intensity.

In conclusion it is possible to say that CH and C_2 radicals are mainly concentrated in the internal core of flame and that this is properly the combustion zone.

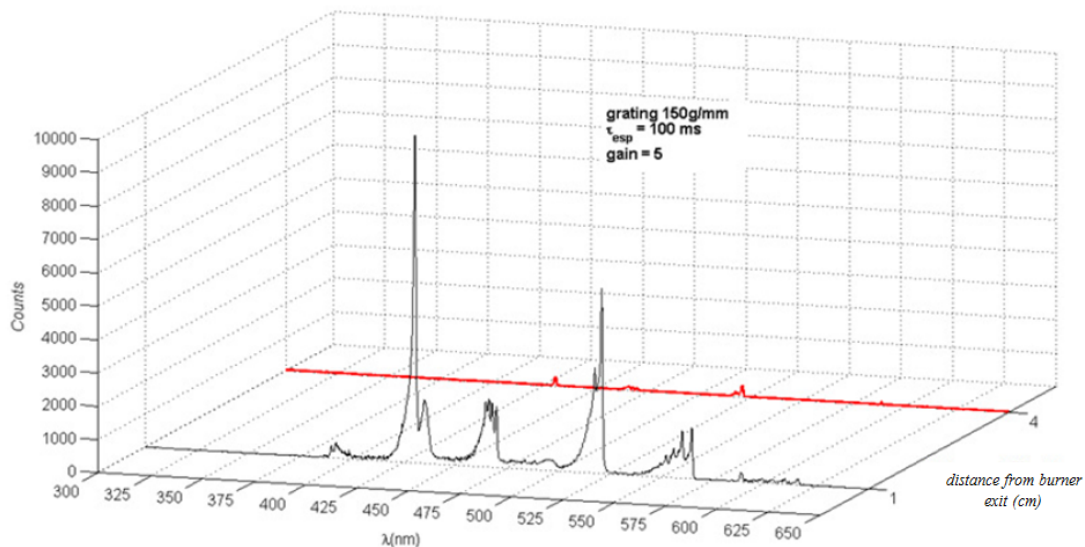


Fig. 11 Spectra of premixed flame along axial direction of flame at 1cm and 4cm from burner exit, grating 150 g/mm, exposure time 100ms and gain 5.

6.3 Comparison between a diffusive flame and a premixed flame

In order to make a comparison between premixed flame spectrum and diffusive flame spectrum it has been acquired the radiation emitted by a diffusive flame (red spectrum in figure 12). Using results just reached about position of combustion zone in a premixed flame, the diffusive flame spectrum has been recorded at 1cm from the exit of the burner. Operating conditions adopted have been the same for both premixed and diffusive flame.

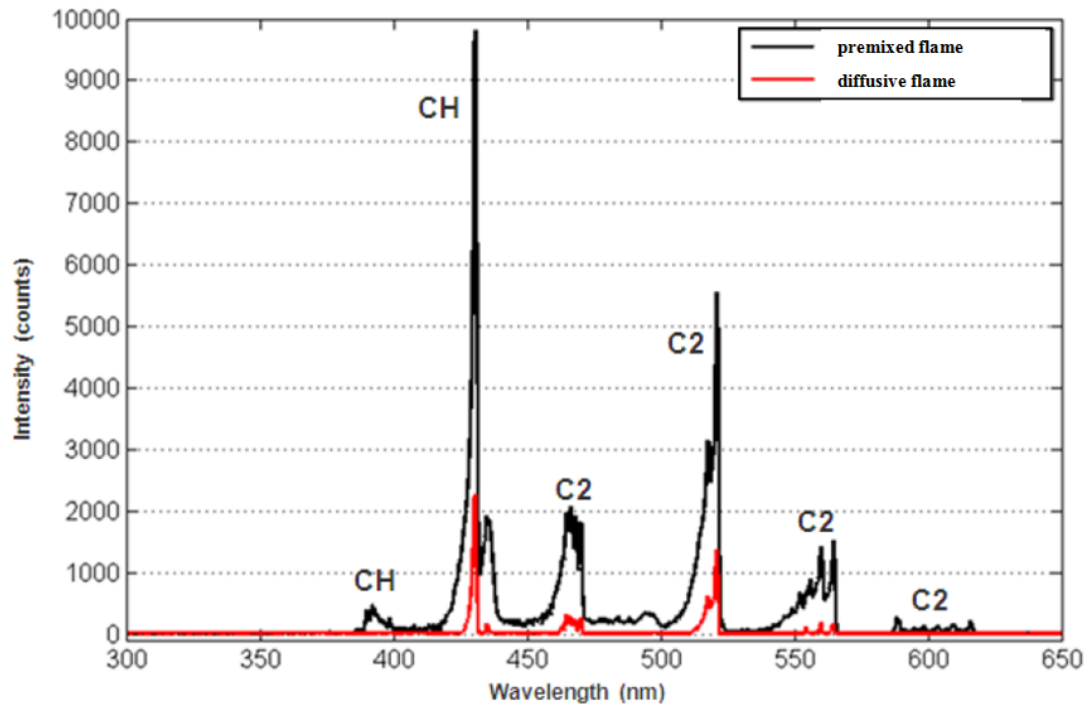


Fig. 12 Spectra of a diffusive flame and of a premixed flame for fixed grating 150 g/mm, gain 5 and exposure time 100ms.

Comparing the two spectra in figure 12 it is possible to observe that the premixed flame spectrum shows more intense bands respect to diffusive flame spectrum. It is reasonable to assume that the combustion zone in a diffusive flame is placed at a greater distance from the burner exit respect to a premixed flame. This is caused by the fact that, in diffusive flame, air and fuel are not mixed before combustion reaction so the combustion reaction is delayed along the axial extension of flame.

6.4 Time-dependent measurements

To take advantage of potential of measurement system it has been acquired spectra with acquisition frequency of 1Hz on the premixed flame, with exposure time equal to 100ms and using the grating of 150 g/mm. During acquisition of these spectra the grating can not move to scan the whole wavelength range the monochromator could sweep. The range we can analyse depends on the density grooves of the grating. The scannable range decreases while increasing the density grooves. For this reason, for the acquisitions at a fixed frequency, we chose the grating with 150 g/mm in order to have the maximum wavelength range. In figure 13 are shown spectra of the premixed flame at 1cm from the exit of the burner and with exposure time equal to 100ms with an acquisition frequency of 1Hz.

In the reported spectra there are no appreciable differences in the single emission bands while the time goes. In fact, to appreciate the presence of fluctuations in the combustion area it is necessary to operate at higher frequencies.

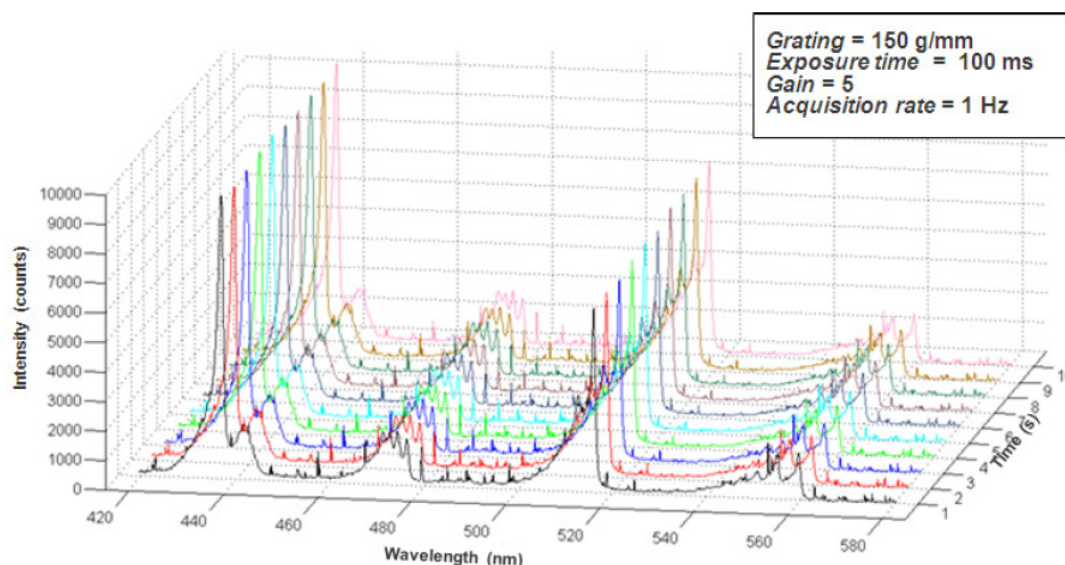


Fig. 13 Time-dependent spectra of a premixed flame for fixed grating 150 g/mm, gain 5, exposure time 100ms with a frequency of 1Hz.

6.5 Data post-processing and flame temperature calculation

Spectra acquired on Bunsen burner have been analysed to identify chemical species emitting in 350 – 650nm and to calculate their temperature. Different software have been used to perform a complete data post-processing: *MatLab* has been used to correct experimental spectra both in intensity and in wavelength, *LifBase* and *SpecAir* have been used to identify chemical species emitting in combustion zone and to calculate temperature of identified emitting radicals. In particular *LifBase* has been used to analyse *CH* emission band while *SpecAir* has been used to analyse *C₂* emission band.

Now it will be described the step-by-step process it has been done to reach the goals just reported.

6.5.1 Correction of experimental spectra with *MatLab*

Experimental spectra can typically experience a shift in wavelength respect to expected value and not correct relative intensities of emission bands because of non-linear response of measurement chain. For these reasons *MatLab* has been used to make some corrections about experimental spectra as follows:

1. import of experimental spectra in *MatLab* in *txt* format;
2. calculation of experimental spectra shift respect to reference spectra (calibration in wavelength);
3. calculation of the efficiency curve (calibration in intensity);
4. corrections of the experimental spectrum for both shift in wavelength and measurement chain efficiency.

6.5.2 *CH* radical temperature calculation through *LifBase*

LifBase software has been designed to give all information about transitions of *OH*, *CH* and *NO* diatomic molecules coming from probability calculations.

Thanks to the presence in *LifBase* database of hydrocarbon derivatives species like *CH* it is possible to generate emission spectra of this chemical species at different temperatures.

All post-processing analysis have been done on spectrum in figure 14. This figure shows the normalized and corrected (in wavelength and in intensity) experimental spectrum which has been analysed in *LifBase* and *SpecAir* to identify chemical species and to calculate their temperature. The experimental spectrum has been acquired in the following operating conditions: 150g/mm grating, exposure time $\tau_{exp} = 100\text{ms}$ and *gain* = 5.

The first operation which has been carried out in *LifBase* was the simulation for different temperatures of emission spectra of *CH* radical. Spectra have been generated one by one in *LifBase* and then they were placed

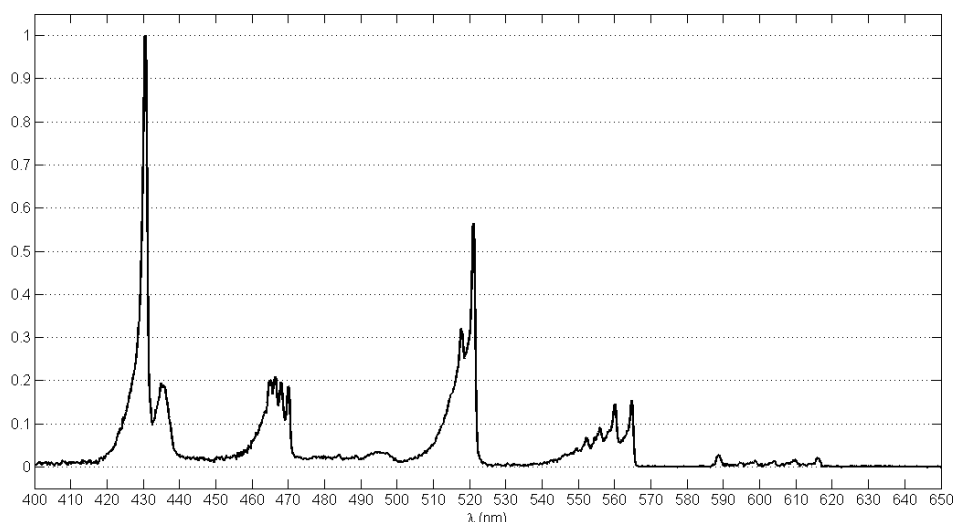


Fig. 14 Normalized and corrected (in wavelength and in intensity) experimental spectrum. This is the spectrum analysed in *LifBase* and *SpecAir* to identify chemical species and to calculate their temperature. This experimental spectrum has been acquired in the following operating conditions: 150g/mm grating, exposure time $\tau_{exp} = 100\text{ms}$ and gain = 5.

on a single chart in *MatLab* together with normalized experimental curve (Figure 15).

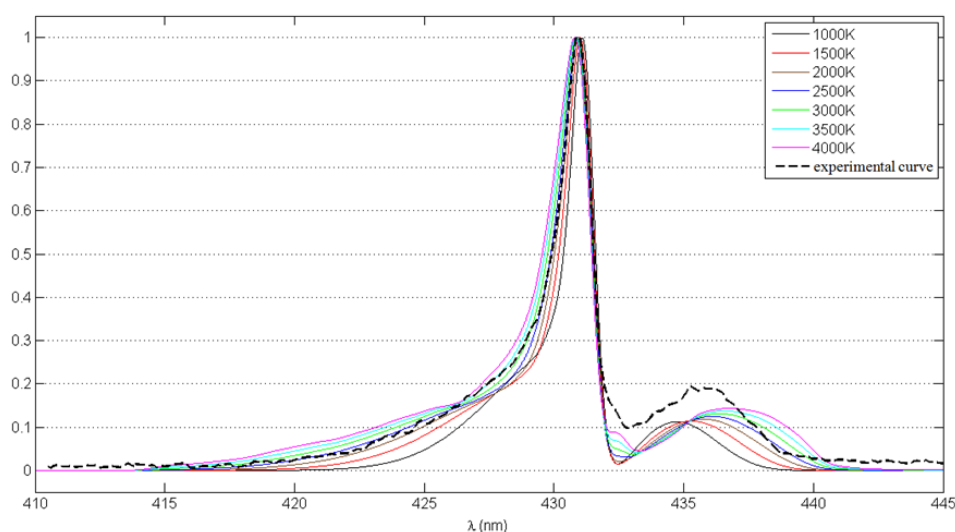


Fig. 15 Normalized spectra of *CH* radical for different temperatures going from 1000K to 4000K with step 500K.

From a visual comparison it might be noticed that experimental curve is positioned between the theoretical curves corresponding to 2500K and 3000K. This suggests to focus the attention on this temperature range. In order to refine temperature approximation other spectra have been generated in the range between 2500K and 2900K with step 50K. As done before, these spectra have been compared with the experimental one (Figure 16). In order to make clearer the graph, curves in figure 16 are with step 100K instead of 50K.

LifBase does not contain a specific routine to perform the curve matching between the theoretical spectra and the experimental spectrum. To overcome this problem it has been written a *MatLab* script to calculate the distance function between the experimental curve and the theoretical curves in the established range of temperatures.

It should be noted that comparison between the theoretical spectra and the experimental spectrum has been done only on the first band (up to about 432nm) and not on the right shoulder of curve (from about 432nm onwards). That is because the latter band is the result of the emission of both radicals *CH* and *C₂*.

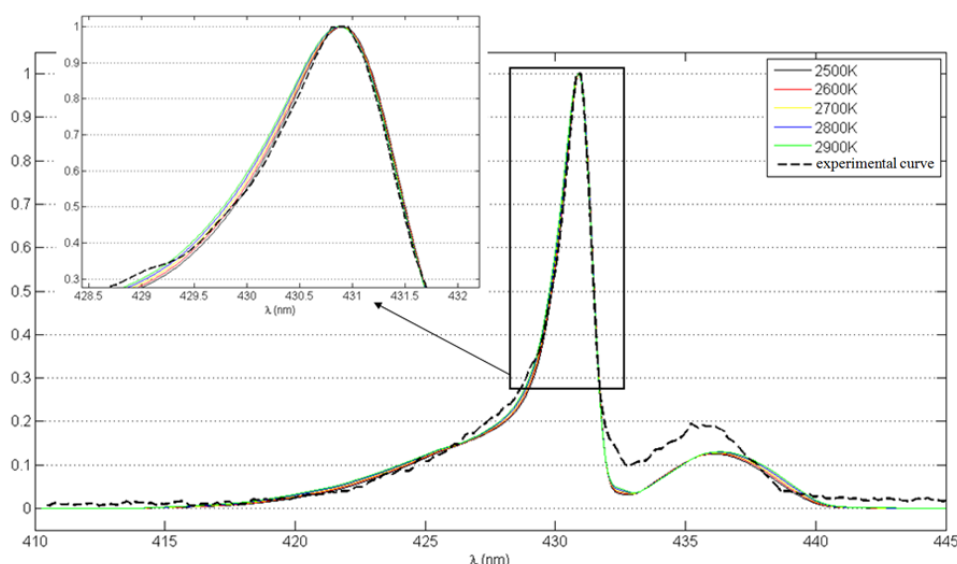


Fig. 16 Comparison between experimental curve and theoretical curves generated in *LifBase* for different temperatures varying from 2500K to 2900K with step 100K.

The minimum deviation of theoretical curves from the experimental one is at the temperature of 2750K.

6.5.3 C₂ radical temperature calculation through *SpecAir*

SpecAir is a specific software to analyse spectra emitted by plasmas. Thanks to the presence in the database software of hydrocarbon derivatives species such as radical C₂, it is possible to generate emission spectra of such chemical species. These spectra have been then compared with the experimental spectrum to calculate temperature of emitting radical.

Analysis with *SpecAir* has been performed band by band in order to obtain more accurate values of temperature. In fact, corrections made by software for a band could be not relevant for another band.

The first thing to do in *SpecAir* to post-process data is to import *slit function*: a Gaussian function which acts as a filter on the generated spectrum to simulate slit width of monochromator used and density grooves of the used grating. After this operation the experimental spectrum can be analysed with *SpecAir* embedded tools.

The most powerful tools of calculation in *SpecAir* are *Find Transition* and *Fit to Spectrum*. The first tool lets find transitions present in experimental spectrum. This is made automatically by the software comparing all basic spectra present in its database with the experimental spectrum. Once found the transition it is known the radical emitting in the band under analysis. The latter tool, *Fit to Spectrum*, is more accurate than the previous one. This tool finds a constrained minimum in the distance function between experimental spectrum and theoretical ones. The output is the temperature of emitting radical with accuracy fixed by user.

The temperature of the combustion zone carried out has been obtained calculating the arithmetic mean between the four values of temperature: 2750K, 2906K, 2695K, 2731K. Then it has been measured the maximum distance from the mean value σ . The calculated temperature can be summed up in the following expression: $T = \bar{T} + \sigma = 2771 \pm 135\text{K}$.

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