Diagnosis of Carbon dioxide as Combustion Products of Gasoline Engine Using Laser Induce Fluorescence (LIF) Technique Modeled by Python program

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Abstract:- *This work is aimed to diagnosis the gasoline engine products using laser induce fluorescence technique modelled by python language. The software developed allows us to diagnosis the gasoline combustion products in terms of fluorescence, quantum efficiency, pressure of the emission, and lifetime. In the simulation model the temperature, the vacuum chamber thickness, the weight ratio in gram units of the combustion gas, and the molar absorbtivity were allowed to be varied for the all of gasoline combustion products (CO_x, NO_x, H_2O, Ni and H-C). From the simulation samples of the results of the laser induce fluorescence from Nd: YAG (266 nm) laser source were presented and discussed. The samples of the carried results showed that the Python software developed to study the emission of the combustion products such as CO_2 sample from the gasoline engine is in a good agreement with the literature work.*

Keywords: *Gasoline engine: LIF (laser induces fluorescence): combustion products: Python language*

1. INTRODUCTION:

Laser-based detection of combustion species has been proven an important tool for combustion research [1]. There are a number of laser related techniques to study combustion processes, namely, laser induced fluorescence (LIF), Raman Spectroscopy, and Rayleigh scattering [2]. The recording of fluorescence radiation of molecules excited by ultraviolet (UV) optical radiation is common practice in the chemical analysis of organic components. The advent of powerful lasers providing radiation at UV wavelengths allows this technique also to be used in engines. Furthermore, the narrowband tuning capabilities of excimer lasers have opened the path to LIF of specific molecular species present in the combustion process 3]. The analysis of transfer paths and transfer probabilities gives a clear indication of how the fluorescence signal is influenced by the irradiating field (spectral irradiance), the molecular properties (population density, absorption, transfer and emission probabilities, dissociation) and the molecular environment (energy transfer concurrent to fluorescence radiation, collisional quenching). For molecules such as H_2, H_2O, NH_3, and CO that do not have accessible excitation frequencies in the UV/visible region but have resonances in the vacuum ultraviolet (VUV) region, i.e., wavelengths between 100 and 200 nm, two-photon LIF can be used to reach the desired energy level of the molecule [4]. W.G. Bessler et al. in 2003 investigated the Laser-induced fluorescence (LIF) of carbon dioxide with excitation between 215 and 255 nm with spectrally resolved detection in 5–40 bar premixed $CH_4/O_2/Ar$ and CH_4/air flat-flames at fuel/air ratios between 0.8 and 1.9. They found that the LIF signal consists of a broad (200–450 nm) continuum with a faint superimposed structure, and this signal is absent in similar $H_2/O_2/Ar$ flames. They concluded that there is strong evidence this signal arises from CO_2, as the signal variations with excitation wavelength, equivalence ratio and flame temperature all correlate with CO_2 absorption cross-sections, and they showed that signal is linear with pressure and laser fluence within the investigated ranges [6]. In (2013) Joakim Rosell et al. presented an investigation of three excitation/detection schemes for two-photon excitation laser-induced fluorescence on carbon monoxide. The schemes are evaluated for pressure and quenching partner dependencies and C_2 interference. In this work we use the python language to model and simulate the laser induced fluorescence (LIF) of the gasoline combustion products by using python language. Due to its advantages and high detection accuracy LIF are a subject of a heavy researches. Many parameters that influences the detection of the LIF signal of the combustion products are important in investigation of the gasoline combustion products, the type of the molecule, its properties such as (molecular weight, concentration, absorbtivity, the length the combustion engine, etc.), the most common emission encountered in the combustion of the gasoline are CO_2, CO, NO_x (x= integer), and HO, the emission fluorescence intensity, life time, quantum efficiency and peak emission are important to be considered in addition to the excitation wavelength in the LIF [3]. In this article we use the modelled LIF calculation software written using python language to study the fluorescence emission lifetime against wavelength as a function in temperature, quantum efficiency versus laser wavelength as a function of temperature, fluorescence versus wavelength as a function of the weight ratio, and the fluorescence versus $P_{emission}$ as a function of weight ratio for the CO_2 gasoline combustion products, and to study the relation between the fluorescence intensity and the temperature.

2. MODELING OF THE LIF USING PYTHON:

The governing process equations to be modelled are:

First: the quantum efficiency, of photochemical reaction which is expressed by: $E = h\nu$; and using the relation between frequency and wavelength:

$$v = \frac{C}{\lambda} \qquad (1)$$

where C is the speed of light in vacuum, using a laser 266 nm in this study as it's a widely used wavelength in experimental works of LIF [7]. Then the frequency can be calculated.

Second: the initial intensity of the emission which is given by:

$$I_0 = \frac{2v^2 K_B T}{c^2} \qquad (2)$$

And from the fact that the $number \quad mole = \frac{weight}{molar \quad mass}$; so the number of decomposed molecules can be expressed as $N. \; of \; molecules \; decomposed = N.of \; mole \times N_A$ (3)

Therefore the number of photons absorbed will be:

$$number \; of \; photons \; absorbed = I_0 \frac{\lambda}{hc} t \qquad (4)$$

$$\phi = \frac{Number \; of \; molecules \; decomposed / formed}{Number \; of \; photons \; of \, radiation \; energy \; absorbed}$$

The absorption equation is:

$$A = \varepsilon_m \times L \times c \qquad (5)$$

Where ε_m is the molar absorbtivity, taking the fact that the molecular molar absorbtivity's are in the range ($3 \times 10^8 - 3 \times 10^5) M^{-1} cm^{-1}$; and the concentration can be calculated from:

$$Concentration = \frac{Weight}{Molar \quad mass} \times \frac{22.414}{1.6} \qquad (6)$$

Finally the equation that describes the fluorescence is given by [8]:

$$F = I_0 \times \phi \times A \qquad (7)$$

The black body radiation law can be used to model and calculate the $P_{emission}$, first we must calculate the emissivity from:

$$E(\lambda, T) = \frac{2\pi hc^2}{\lambda^5} \times \frac{1}{e^{(hv/KT)} - 1} \qquad (8)$$

$$\varepsilon = \frac{E(\lambda)}{E(\lambda, T)} \qquad (9)$$

Where $E(\lambda)$ represent the real body energy at the same wavelength, and $E(\lambda, T)$ is the black body energy at the same wavelength and temperature. Then the equation of the $P_{emission}$ is:

$$P_{emission} = \frac{\varepsilon \sigma}{c} T^4 \qquad (10)$$

The last is the lifetime, and we need to calculate the viscosity of the gas to calculate it, and the equation of viscosity:

Viscosity of Gases: η

$$\eta = \eta_0 + \alpha t - \beta t^2 \qquad (11)$$

Where η is the viscosity of the gas at t ^oC in poise, η_0 is the viscosity of the gas at 0 ^oC in poise, and *t = temperature*, and α *and* β are constants; $\alpha = 0.56 \times 10^{-7}$ and $\beta = 0.1189 \times 10^{-9}$

Table (1) shows the physical properties of the products of the gasoline combustion which needed to be studied via LIF modelled using Python language.

Table (1): *Physical properties of the gasoline combustion products:*

Name	***Formula***	***Molar mass***	***Viscosity of gas at t c poise***	***Radius (m)***
Carbon dioxide	CO_2	44.0095	0.00013830126	165×10^{-12}
Carbon monoxide	CO	28.0101	0.00016483165	188×10^{-12}
Nitrogen	N_2	28.0134	0.0001781	132×10^{-12}

$A = \varepsilon_m \times L \times c$

Nitric oxide	NO	30.0061	0.00011584498	158×10^{-12}
Nitrogen dioxide	NO_2	46.005	0.00010254	151×10^{-12}
Water	H_2O	18.0153	0.00016531187	132.5×10^{-12}
Hydrocarbon	HC	13.0186	0.00012025	146×10^{-12}

Table (2) shows the typical time scales of the process, neglecting quenching by external molecules, which were used in the study of the fluorescence of gasoline combustion products in the developed software.

Table (2): *Process outside the gasoline combustion engine and a typical time scales:*

Process	***Time scale***
Internal conversion	$10^{10}-10^{14}S^{-1}$
Fluorescence	$10^{7}-10^{9}S^{-1}$

The following figure (1) shows a schematic diagram of the flow chart of LIF in python:

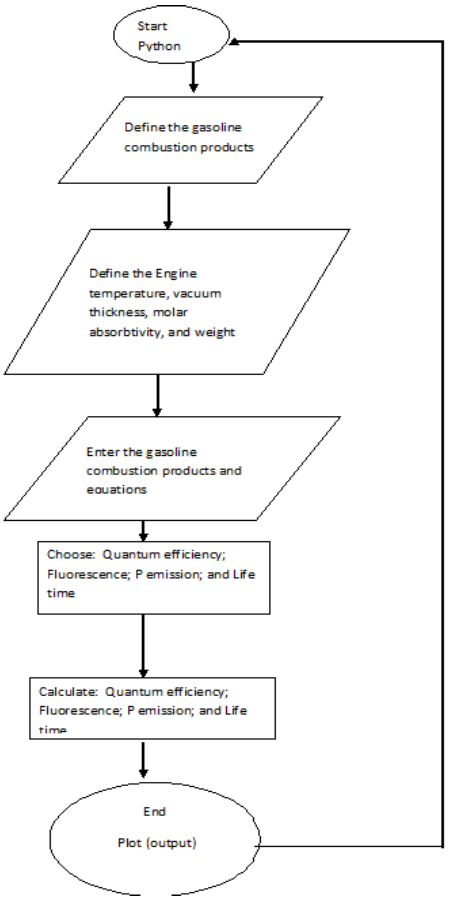

Figure (1): LIF flowchart in python

Figure (2, a) shows the LIF software developed user interface.

Figure (2, a): The Python developed LIF simulation user interface

The first icon shown in figure (2, a), illustrates the entry and build the output of the LIF of the gasoline combustion product calculation interface, s shown in figure (2, b).

Figure (2, b): LIF of gasoline combustion calculation interface

3. RESULTS AND DISCUSSION:

The developed LIF calculation software of the gasoline combustion products was used to study the (i) fluorescence emission lifetime against wavelength as a function in temperature, (ii) quantum efficiency versus laser wavelength as a function of temperature, (iii) fluorescence versus wavelength as a function of the weight ratio, and (vi) the fluorescence versus $P_{emission}$ as a function of weight ratio. Figure (3.1, a, b, c and d) shows the results of (i), (ii), (iii), and (iv) for the carbon dioxide.

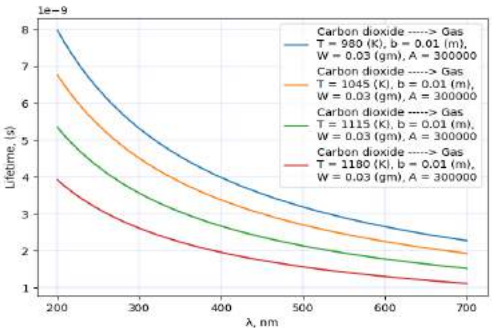

Figure (3.1, a)

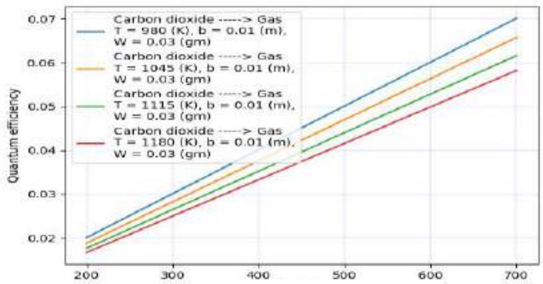

Figure (3.1, b)

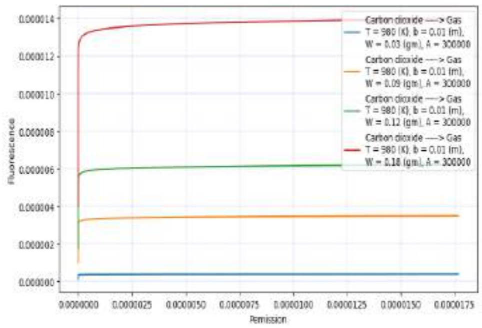

Figure (3.1, c)

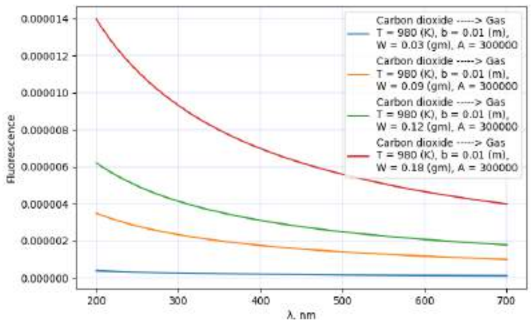

Figure (3.1, d)

Figure (3): (a) fluorescence emission lifetime against wavelength as a function in temperature, **(b)** quantum efficiency versus laser wavelength as a function of temperature, **(c)** fluorescence versus wavelength as a function of the weight ratio, and **(d)** the fluorescence versus Pemission as a function of weight ratio of the carbon dioxide gasoline combustion product

As the results showed in figure (3.1, a) the fluorescence emission lifetime of the carbon dioxide is exponentially decay, and it decrease with wavelengths as a result of the temperature increase; while the weight, the thickness of the vacuum chamber, and the molar absorbtivity are kept fixed. Also a similar discussion can be said for the quantum efficiency shown in figure (3.1, b) in which the quantum efficiency increased with the wavelengths and when the temperature are increased while the weight ratio and the vacuum thickness remains fixed, the quantum efficiency curves decrease downwards. In Figure 4.1,c, showed the fluorescence intensities of the carbon dioxide versus Pemission for different weight ratios (0.03, 0.09, 0.12, and 0.18) gm at T = 980 K as shown on the bottom left, it's clear that increasing the weight ratio results in an increase in the fluorescence. This is in a good agreement of the work of Jochen Scholz et al. in (2006) [9]. Figure (3.1, d) shows the fluorescence of the carbon dioxide against the excitation wavelengths, the results showed that the fluorescence is exponentially increased as the weight ratio is increase while molar absorbtivity, thickness of the vacuum chamber and the temperature were kept fixed. Figure (3.2) shows the carbon dioxide gasoline combustion product fluorescence.

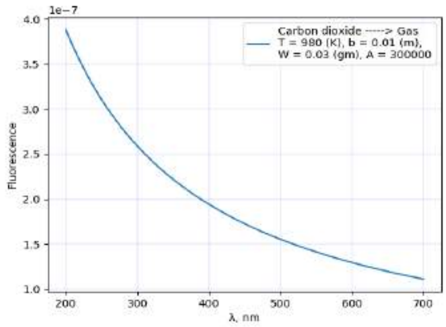

Figure (3.2): Fluorescence of carbon dioxide gasoline combustion product

The CO_2-fluorescence signal is strongly dependent on excitation wavelength and showing to be decrease with increasing the wavelength as shown in figure (3.2), this agree with the work of W.G. Bessler et al. (2003). The dependence of the fluorescence on the excitation wavelength is in qualitative agreement with theoretical knowledge of the wavelength dependence of the CO_2 absorption cross-section.

Figure (3.3) shows the fluorescence intensity against wavelengths as a function of temperature for the carbon dioxide.

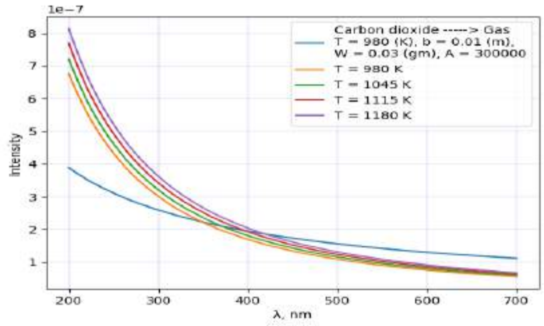

Figure (3.3): Fluorescence intensity of carbon dioxide gasoline combustion product

It is clear that the fluorescence intensity curve increased (or shifted up) as a results of the temperature increase, the point of intersection of the fluorescence and intensity gives the exact intensity and the wavelength at specific temperature, taking this into account the figure (3.3) proved that as a result of the increase in the temperature the fluorescence intensity decease while the fluorescence increase for the case of carbon dioxide gasoline combustion product, i.e., temperature dependence of the fluorescence emission intensity [10].

4. CONCLUSION:

The python language was used to model the LIF of the gasoline combustion products using the governing equations successfully, the article presented the results of the Carbon dioxide (CO_2) gasoline combustion only, but the software built to investigate the rest of the gasoline combustion products such (CO, NO, NO_2, N_2, H_2O, and HC), the built LIF simulation software was in good agreement with the experimental data of LIF for gasoline combustion products. In conclusion, the fluorescence emission lifetime against wavelength as a function in temperature, quantum efficiency versus laser wavelength as a function of temperature, fluorescence versus wavelength as a function of the weight ratio, and the fluorescence versus $P_{emission}$ as a function of weight ratio was studied using the build LIF simulation for the CO_2 gasoline combustion products. And it was found that the fluorescence intensity decrease while the fluorescence wavelength increase when the temperature is increased for the case of carbon dioxide gasoline combustion product.

REFERENCES

[1] RAFEEF ABU-GHARBIEH *(2001), Laser Sheet Imaging and Image Analysis for Combustion Research, (PhD thesis), School of Electrical and Computer Engineering Chalmers University of Technology, downloaded from: https://pdfs.semanticscholar.org/1bf3/33b423c846e25f7df53c8c93512c39ce904a.pdf*

[2] T. K. Subramaniam (2015), *Analysis of Internal Combustion Engines Using Laser Induced Fluorescence Spectroscopy, AASCIT Journal of Physics, Volume 1, issue 4, pp. 288-291*

[3] Christian Brackmann et al. *(2004), Laser-induced fluorescence of formaldehyde in combustion using third harmonic Nd: YAG laser excitation, Spectrochimica Acta Part A Molecular and Biomolecular Spectroscopy, Volume 59, issue 14, pp. 3347-56*

[4] Joakim Rosell et al. *(2013), Comparison of Three Schemes of Two-Photon Laser-Induced Fluorescence for CO Detection in Flames, SAGE Journals, Applied Spectroscopy, Vo*lume: 67 issue: 3, page(s): 314-320, https://doi.org/10.1366/12-06704

[5] W.G. Bessler et al., (2003), Carbon dioxide UV laser induced fluorescence in high-pressure flames, Elsevier, Chemical Physics Letters 375,pp.344-349, doi:10.1016/S009-2614(03)00858-3

[6] Gao Star et al. (2015*), Laser Induced fluorescence of fused silica irradiated by KrF laser, The Proceedings of SPIE - The International Society for Optical Engineering 9532, DOI: 10.1117/12.2186063*

[7] Luke Thompson *(2015), Planar Laser Induced Fluorescence Experiments and Modeling Study of Jets in Cross flow at Various Injection Angles, (Master Thesis University of Central Florida), Electronic Theses and Dissertations, 1434, http://stars.library.ucf.edu/etd/1434*

[8] De Sercey, *Guillaume, (2004), Laser induced fluorescence for the measurement of air-to-fuel ratios in gasoline direct injection engines, (PhD thesis), University of Brighton, ISNI: 0000 0001 3420 6275*

[9] Jochen Scholz *et al. (2006), Verification and Application of Fuel- Air-Ratio-LIF, 13th Int Symp on Applications of Laser Techniques to Fluid Mechanics Lisbon, Portugal, 26-29 June, 2006 #1256*

[10] Christopher J. Ellison and John M. Torkelson *(2002), sensing the glass transition in thin and ultrathin polymer films via fluorescence probes and labels, Journal of Polymer Sciences: Part B: Polymer Physic, volume 40, pp.2745-2758*

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