DETERMINATION OF HOT GAS TEMPERATURE PROFILES BY IR SPECTROSCOPY

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ABSTRACT: Determination of exhaust gas temperature and concentration is a critical point for the study and the optimization of engines combustion. A non-invasive method has been developed based on the analysis of the CO2 infrared spectrum, which is particularly sensitive to the temperature between 4.16 µm and 4.20 µm [1]. Inversion of the radiative transfer equation ensures the retrieval of temperature and concentration profiles, from transmission or radiative intensity measurement and complementary information about the profiles shape. The inverse problem is solved by minimizing the quadratic difference between the measured spectrum and the calculated one from the spectroscopic data listed in HITRAN-08 [2] [3] [4]. This method has been validated on a flowing CO_2/N_2 gas mixture heated up to 300°C. Identified temperature has shown good agreement with the one recorded by thermocouple: difference was less than 2.5%. This optical technique, without medium disturbance, may be used in various applications involving combustion, such as the study of Diesel exhaust pipe.

INTRODUCTION.

Temperature is a critical information on thermodynamic systems. In the specific case of combustion, the energetic or running optimization of systems is strongly linked to this parameter since their efficiency is directly proportional to the temperature. Environmental standards regularly impose stronger reduction of pollutants or greenhouse gas emission to the automotive industry. An additional solution to all the pollutant filtering or transforming systems such as particles filters or catalytic converter is to improve engine efficiency. In order to make such improvements, the solutions must be experimented while designers have to minimize trials and prototypes. Currently, some numerical tools are developed and their validation must be achieved by comparisons with experimental values. In this paper, a new method to determine temperature and gas concentration profiles in thermodynamic systems is proposed. This original non-invasive method has been developed as part of a research project on the engines air-loop for automotive industry: SIMBA. The resulting numerical model concerns the whole gas circulation in the engine from the inlet to the exhaust lines. Inlet pipes, turbocharger, coolers, cylinders, exhaust and EGR lines have been taken into account for the Diesel engine that has been studied. The presented method is based on the analysis of the CO_2 infrared spectrum, which is particularly sensitive to the temperature between 4.16 µm and 4.20 µm [1]. The inversion of the radiative transfer equation from transmission or radiative intensity measurements ensures the retrieval of temperature and concentration profiles. Finally, the method is applied to the exhaust of a DV6-TED4 PSA engine.

RADIATIVE PROPERTIES OF GAS AND PRINCIPLE OF THE METHOD.

The properties of the infrared radiations emitted by a hot gas are entirely different from those emitted by a hot solid surface.

According to the Planck's law, the radiative intensity emitted by a blackbody is a function of temperature and wavelength (here the wavenumber σ):

$$L_\sigma^O(\sigma,T) = \frac{C_1.\sigma^3}{e^{\frac{C_2.\sigma}{T}} - 1}\ (W.cm^{-2}.sr^{-1}.cm)$$

where T is the temperature of the body (K), σ the wavenumber (cm^{-1}), $C_1 = 1.191E^{-12}$ (W.cm^2.sr^{-1}) and $C_2 = 1.438$ (K.cm). Usually, the wavelength λ of the radiation is given in µm but for IR spectroscopy, the conventional unit of the wavenumber σ is cm^{-1}. The wavenumber is given by the following formula: $\sigma\ [cm^{-1}] = {10000}/{\lambda[\mu m]}$.

Blackbody's law is represented on the following figure at 300K, 500K, 700K and 900K in the spectral range 0 cm^{-1} to 6000 cm^{-1}.

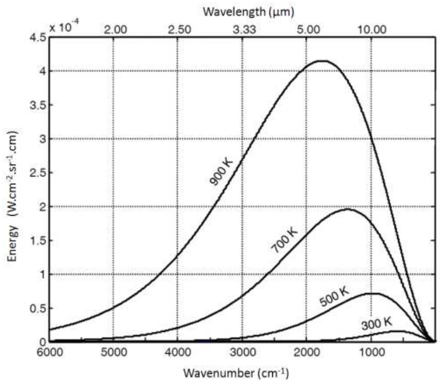

Fig. 1 : *Energy emitted by a black body for various temperatures*

On the contrary to a hot solid medium which emits radiations on a continuous spectrum, a hot gas emits radiations only on discrete wavelengths (and conversely, a cold gas absorbs radiations only on discrete wavelengths and not on a continuous spectrum). For a gas, the radiative emission or absorption is directly linked to the molecular energy level which can be divided in four types: kinetic energy, electronic energy, vibrational energy and rotational energy. Besides, these discrete wavelengths are gathered in wavelength stripes, whose width increases as the temperature, the concentration and the pressure of the gas rise. The infrared lines of carbon dioxide spectrum present an important dependence to temperature around 2400 cm^{-1}. Therefore, this molecule is the main gas of this study. When torque and rpm increase in an engine, the temperature and concentration of carbon dioxide increase in the exhaust gas. A Fourier Transform Infrared spectrometer (FTIR) can give really accurate information about this kind of lines and the following figure illustrates this point with carbon dioxide absorption lines measured on the exhaust gazes of a DV6 Diesel engine:

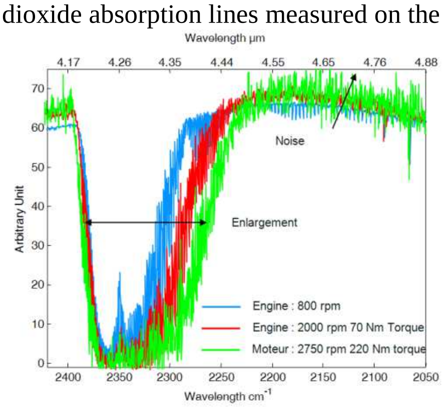

Fig. 2 : Typical gas absorption lines for carbon dioxide in the infrared.

As expected, temperature and concentration of CO_2 increase into the exhaust gases. The shapes of the spectra are modified and the absorption lines are getting larger. The shape and intensity of gas absorption or emission lines are deduced from the gas temperature and concentration data along the optical axis "x". At the wavenumber "σ" the transmission is given by:

$$\tau_\sigma(x) = e^{-K_\sigma(x,T,C).dx}$$

where, K_σ is the monochromatic absorption coefficient of the gas. For a gas volume, this expression can be integrated from x =0 to x= d with "d" the thickness of the system as shown on the following figure:

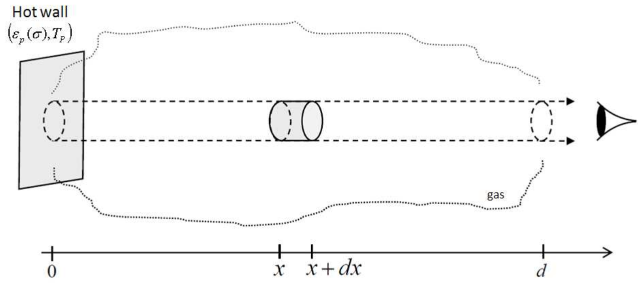

Fig. 3 : Typical experimental configuration.

Then, the radiation emitted by this specific volume is given by the following form of the integrated radiative heat transfer equation:

where, is the monochromatic transmission of the gas from “x” to “d” given by:

Since the radiation can be defined by:

and finally:

With this last equation, the radiative heat transfer equation may be solved numerically assuming that the heterogeneous and nonisothermal gas volume can be divided in small elements. For each of them, the properties are considered homogeneous and the temperature constant. Thus, a system divided into “N” elements of constant thickness “e = d/N” and containing carbon dioxide, is here considered as shown below:

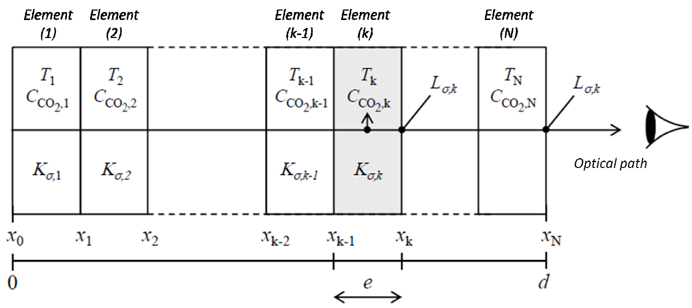

Fig. 4 : Heterogeneous system divided into N homogeneous and isotherm elements.

Here, k = 0 indicates the origin of the radiation in the system. It may be null or bounded by a hot plate characterized by an emissivity “ε(σ)” and its temperature “Tp”. The energy emitted by this element is defined as . Of course, the discretization of the temperature and concentration profiles for this system is necessary. It is assumed here that for each element, the temperature and concentration of gas are constant values attributed at the center of the element and calculated by:

and

Using the temperature and concentration calculated for each element, the corresponding value of the monochromatic absorption coefficient may be computed by an adequate model: [7]. Then, at the end of an element "k", " " may be calculated with this coefficient and the emitted radiation from the previous element :

And finally:

With "N" iterations (k=1,…,N) the radiative intensity emitted at the end of the gas volume may be calculated. The initialization can be done in the case of a hot plate as shown on Fig. 3 with the following value: .

Note that the total transmission factor of the whole volume is .

If spectral measurement are proceeded on a real system, it is possible to find the best parameters for "Tk" and "Ck" to fit the recorded data with the synthetic values. The final result has to be with the monochromatic radiative intensity calculated at the end of the system for the wavenumber (direct problem), and the measured one for the same wavelength. Assuming some properties on the shape of the temperature and concentration distribution discards non-physical results and these profiles can be recovered. As previously indicated, carbon dioxide lines in the infrared present important temperature dependence around 2400 cm^{-1}. In this spectral range, an inverse problem is solved by minimizing the quadratic difference between the measured spectrum and the calculated one from the spectroscopic data listed in HITRAN-08 [2] [3] [4] with the developed model. The minimization code gives the best solution for:

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where, "m" stands for T and C parameters vector. Of course, some parameters are necessary to find the best solution in good conditions. The total pressure of the gas must be known, the boundary conditions (hot plate properties, air thickness between the gas volume and the detection system, spectral response of the optical system), and an assumption about the shape's distribution of both temperature and concentration must be included as input data. Finally, the following diagram describes the principle of the optimization code:

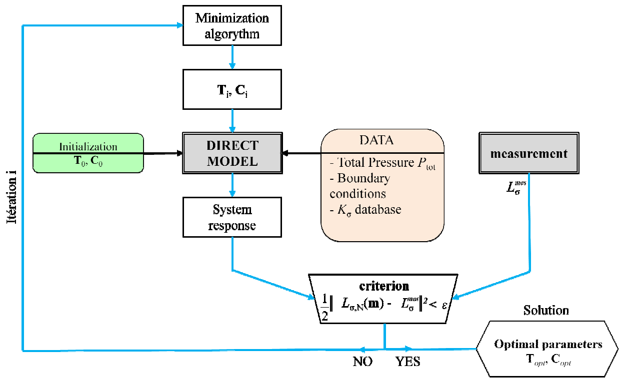

Fig. 5 : Principle of the optimization code.

The validity of the monochromatic values calculated has been verified with a specific gas characterization cell.

INVERSION OF THE GAS VOLUME TRANSMISSION SPECTRUM.

The method has been validated on a synthetic gas bench where the concentration and the temperature of gas were controlled values. A FTIR spectrometer was used to realize transmission measurements on the gas volume. The following figure illustrates the experimental setup:

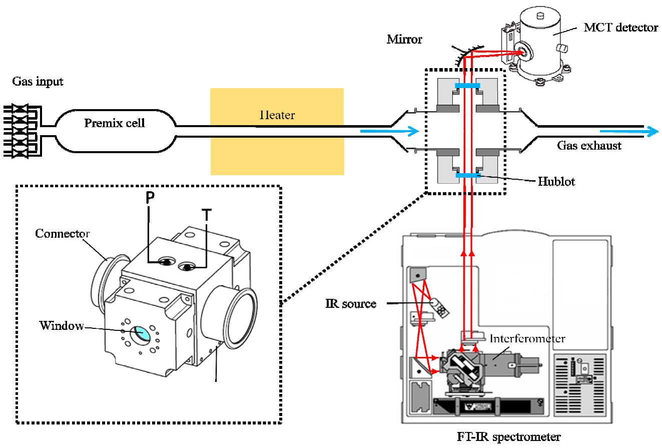

Fig. 6 : Experiment setup on synthetic gas bench for measurement of the transmission spectrum.

The gas mixture flows through a pipe form the premix cell to the measurement cell. A heater controls the gas temperature. Firstly, nitrogen, a neutral gas within the studied spectral range (no absorption in the spectral range of interest) is flowing through the system. Using some optics, the light from the radiative source (internal source of the spectrometer) crosses the gas flow and is collected on an MCT detector after modulation in the Michelson interferometer. The result is a reference spectrum for the radiative source . Then, carbon dioxide is added to nitrogen in the premix chamber and flows through a pipe to the measurement cell. A new spectrum is acquired and gives . In addition, a "K type" thermocouple is used to give a comparison point between the result of the minimization code and the real temperature distribution. A Kulite WCT 312 pressure transducer is also used as shown on Fig. 6 to measure the total pressure of the visualized mixture. The last step gives the spectral transmission of the gas mixture by the calculation of the ratio between the reference spectrum and the spectrum with carbon dioxide:

This transmission measurement doesn't require a global calibration because all the source information and the environment influences are integrated into the reference measurement . Moreover all the environmental perturbations are avoided since the spectrum is determined with the modulated light coming from the Michelson interferometer. Finally, the energy from the infrared source is higher than the self-emission from the gas mixture or from surrounding because the temperature of the internal source of the spectrometer is around 1400K. Furthermore, the radiated energy calculated by Planck's law is about 33 times more important at 1400K than at 600K at 4µm. As the energy of a real body is always lower than that of a blackbody at the same temperature, considering that the infrared source of the spectrometer is close to the blackbody assumptions, this ratio is a minimum value. For all these reasons, the signal to noise ratio is really good in this study and the noticed noise level is about 1%.

The data inversion requires a high resolution spectrum (Fig. 2). Therefore, the acquisition time is quite important: about 4 minutes for a 0.125cm^{-1} spectral resolution. Moreover, the steady state has to be reached before acquiring data. As an example, for a 5%CO_2 and 95%N_2 mixture, the monitoring of temperature and pressure gives the following curves during spectra acquisition:

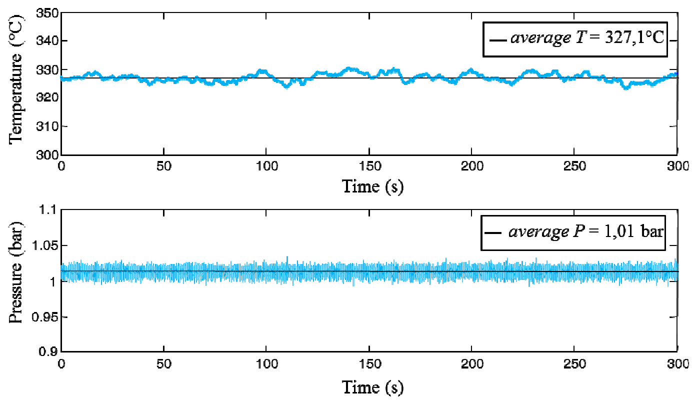

Fig. 7 : Temperature and pressure for a 5%CO_2 and 95%N_2 mixture

Temperature stability is correct and around ±3.6 K which as to be compared to the average value calculated at 600.25 K: the temperature variation is about 0.6% in the standard Kelvin units. Concerning the pressure, the stability is also reached and good. The average value is 1.01 bar, the absolute variation is ±0.02 bar and the pressure variation is about ±1.98%.
For each gas mixture, the average measured temperature value is compared to the retrieved temperature value at the thermocouple's position in the measurement cell. Moreover, as the exact concentration of gas injected in the pipe is known, the result of the inversion for concentration will be compared to this exact value. The results obtained for the identification of temperature and concentration of carbon dioxide for three different cases are presented: first 5%CO_2 / 95%N_2 under 1bar then 5%CO_2 / 95%N_2 under 1.01 bar and finally 10%CO_2 / 90%N_2 under 0.99 bars. For all these tests, the initialization values are T = 300 K, X_{CO2} = 1%. The following tables give the relative differences between calculated and measured values for temperature and concentration:

Molar fraction of CO_2 (%)	5,0	5,0	10,0
T_{tck} (K)	517,3	600,3	441,2
$T_{optical}$ (K)	523,8	607,4	436,5
	1,3	1,2	1,1

Molar fraction X_{CO2} (%)	5	5	10
$X_{CO2,\ optical}$ (%)	4,7	4,9	9,5
	6	2	5

Table 1 : Differences between calculated parameters and real parameters for inversion of transmission measurement.

These results confirm both the measurement method and the data processing of the inversion code.

APPLICATION TO CAR ENGINE: MEASUREMENTS AND RESULTS

Some measurements have been done on the exhaust pipe of a car engine (DV6-TED4; 1.6 HDI; 110 hp). The measurement cell used for the validation of the method on the synthetic gas bench is connected to the exhaust pipe behind a particle filter to prevent obstruction on windows. The experimental setup is described on the following figure and the real position of the cell of the exhaust pipe is shown on the picture:

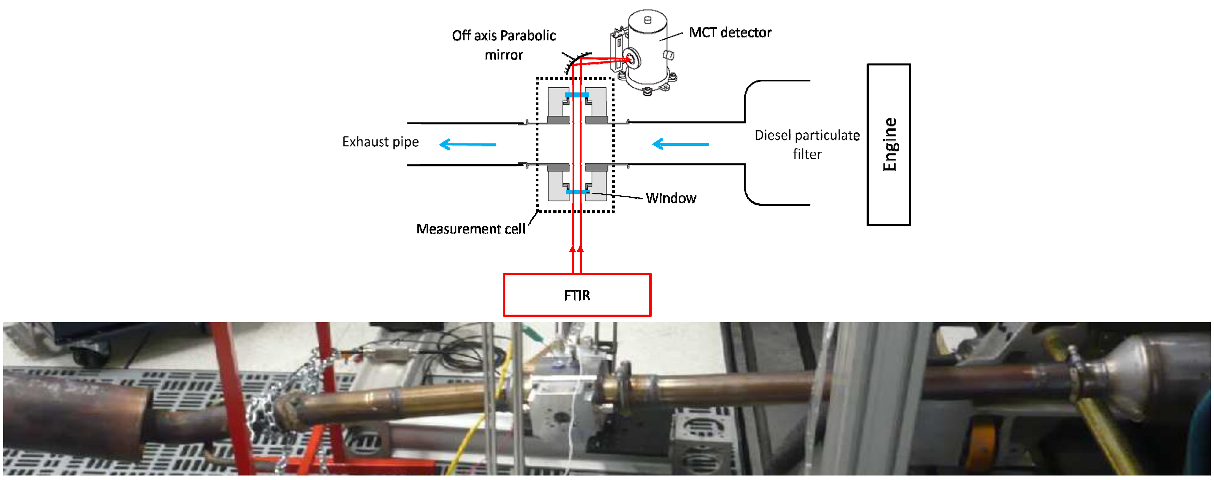

Fig. 8 : Instrumentation set-up for radiative measurement of exhaust gas for a DV6-TED4 Diesel engine

In this experiment, the temperature distribution into the pipe is assumed to fit with a Gaussian curve. Thus the temperature can be parameterized with the equation with . Here is the center position of the Gaussian curve into the pipe, the width of the curve and the temperature asymptotic value. is the temperature difference between the asymptotic value and the center value. The center value is assumed at the center of the pipe . The concentration of carbon dioxide is assumed as constant through the section of the pipe and equal to C_x. So the problem needs the identification of four parameters: , , and C_x.

The presented results are acquired from a 2500rpm engine speed with 40Nm torque. The temperature value from the thermocouple is 590K and the inversion result at the same position gives 601K: the difference between the two values is less than 2%. The molar fraction has been determined at 7.8% and has been compared to the value measured with an industrial FTIR analyzer equals to 7.5%. For this case, the difference on the concentration obtained between an intrusive measurement and the result of the optical method value is less than 3%. On the left side, the following figure shows the measured spectrum, the inversion result and the difference between these values. On the right side, the calculated temperature distribution and the intrusive value for the engine running point is presented.

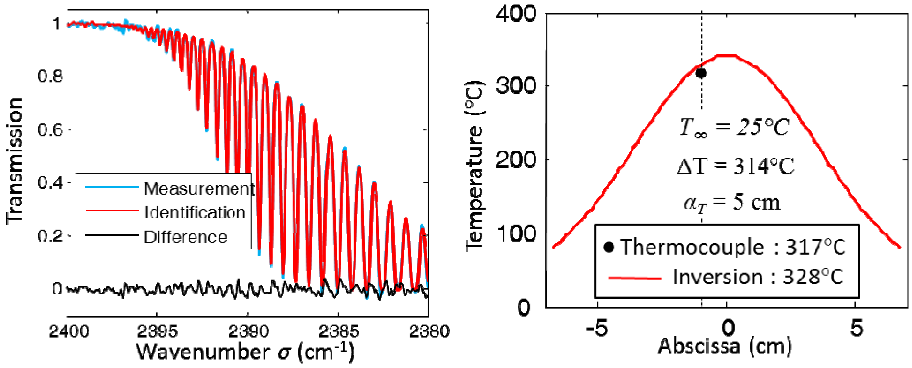

Fig. 9 : Inversion results on the transmission measurement for a DV6-TED4 car engine at 2500rpm and 40Nm torque

The results of the method for this real case are similar to the intrusive data. This study shows that the method is actually relevant for industrial applications. However it has some negative points particularly on the acquisition time and some improvements have to be considered.

CONCLUSIONS AND PROSPECTS

A non-intrusive method has been developed to determine temperature and concentration distributions of a gas volume. The selected species is the carbon dioxide for which the high resolution spectrum of its radiative properties in the infrared bandwidth can be reduced between 2380cm^{-1} to 2400cm^{-1} where an important thermometric effect exists. The analysis of spectral data is achieved thanks to a numerical inversion code especially developed for this application. This code is based on an algorithm which uses local minimization of the radiative intensity gradient value according to the parameters T and C. It ensures rapid convergence to the best solution. For this method, the number of identifiable parameters is limited and it is necessary to assume some particularities about the shape of the distributions. In order to limit the number of parameters, a Gaussian parameterization of the T and C distribution has been assumed instead of searching the value for T end C at each point of the grid. The validation of the method has been done on a synthetic gas bench by inversion of transmission spectra. The inversion of these measures showed a temperature difference reduced at 2.5% with the thermocouple values. The method is applied to carbon dioxide for temperatures under 1000K and near atmospheric pressure but the validity of this method and of the direct model may be extended to other molecules. Moreover, the monochromatic absorption coefficient of CO_2 is done with partition functions given valid up to 3000 K. Thus, the method is not limited to the exhaust of car engines and could be applied to many other systems.

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