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# HT17

## ESTIMATION OF THE TEMPERATURE AND CONCENTRATION DISTRIBUTIONS IN HOT COMBUSTION GASES

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## ABSTRACT

This paper deals with passive optical methods carried out to determine one or two-dimensional temperature and concentration fields $(T,C)$ in semitransparent medium at high temperature. In comparison of common methods using sensors, their main advantage is their non-intrusive feature. The determination of temperature and concentration from the spectral intensity measurements requires using an inversion algorithm adapted to the physical problem. Two cases are presented here: the 1D problem of the estimation of $(T,C)$ profiles of $CO_2$ in exhaust gases of gas turbines, and the 2D problem of two-dimensional $(T,C)$ distributions of $H_2O$ at a cross section of a rectangular ramjet. In each case, the iterative regularization [3] is used to solve the inverse problem of radiation transfer, which is a non-linear Fredholm equation of the first kind.

## INTRODUCTION

The analysis of exhaust gases is important in regard to environmental studies. The determination of temperature fields in combustion chambers is carried out in order to get a compromise: on one hand, an increase of the temperature allows to reach a better efficiency of the engine but on the other hand, it augments the concentration of NOx. Thus, the knowledge of the temperature profile is necessary to develop combustion chamber without hot points generating NOx and also to control combustion directly during the engine operation. Knowing the concentration of polluting components (CO, NOx, UHC) in exhaust gases is also useful to regulate combustion parameters (flow rate, air-fuel ratio…).

Intrusive sensors (thermocouples, extractive probes…) are usually used but they are not often well adapted: a bad resistance at high temperatures, safety problems in combustion chambers. With optical methods, the temperature and concentration fields can be determined without any contact. Some of optical techniques, such as Coherent Anti-Stokes Raman Scattering (CARS [1]) or Laser Induced fluorescence (LIF), permit to measure $(T,C)$ directly. Yet, they aren't easy to put into operation and may be disrupting in industrial combustion. So, their utilization is up to now limited to laboratories studies. We choose to use optical methods based on transmission or emission of radiation in the studied medium. The intensity received by the detector is resulting of the emission, transmission and absorption of the radiation propagating in the considered medium. Thus, an inversion computation is necessary to get temperature and concentration distributions in the gas from the measured spectral intensity (Figure 1). This article deals with two inversion methods used in a one-dimensional case and a two-dimensional application.

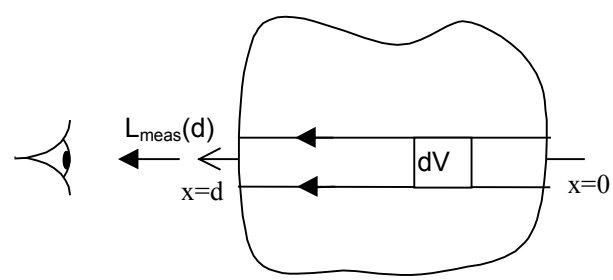



Figure 1: description of the gas medium

## 1. SPECTROMETRY IN HOT GASES

### Inverse problem formulation

The inverse problem is formulated from the equation of radiation transfer in a semitransparent medium. This equation gives the theoretical expression of the spectral intensity transmitted and emitted by the medium. In the 1D case, its expression is:

$$\int_O^d L^0(\lambda_n, T(x)) \frac{\partial \tau(\lambda_n, T(x), C(x))}{\partial x} dx = L_{meas}(d) \quad \text{Eq. (1)}$$

d is the thickness of the gas (Figure 1).

$L_{meas}(d)$ is the measured intensity.

It is a non-linear Fredholm equation of the first kind. To estimate the functions $(T, C)$, the problem is to inverse this equation (1D problem) or a system of two radiative equations (2D problem).

The kernels of the integral,

$$\left| \frac{\partial \tau(\lambda_n, T(x), C(x))}{\partial x} \right| \quad \text{Eq. (2)}$$

are representative of the spatial weight that each part of the gas exerts on the spectral measurement. An element of gas corresponding to an abscise for which the kernel is weak, does not contribute a lot to the measured intensity. The kernel shape indicates from where the information comes.

### Choice of a physical domain

Radiative properties of a chosen component of the gas (spectral transmissivity) are needed as a function of temperature and wavelength. To execute the inversion, it is necessary that the kernels have different behaviors depending on the wavelength. On a range of wavelength, the kernels may overlap. That means kernel informations are correlated. In this case, the different spectral measurements are not independent and the solution of the system is not unique.

### Inversion of the radiative equation

We must minimize a criterion representative of the distance existing between simulation and measured quantity. In 1D and 2D cases, we choose to use the quadratic criterion.

Now, we describe the solution of the inverse problem, first in the 1D case and then in the 2D case.

## 2. ONE DIMENSIONAL INVERSE PROBLEM

In some cases, the access to combustion gas can be difficult or stabilization duration of power settings can be short. So, it is useful to be able to estimate the temperature profile by carrying out only one spatial measurement, which contains several wavelengths.

Here, we propose an inversion method using one spatial measurement and applied to the determination of a temperature profile in exhaust gases.

### Choice of the wavelengths

The wavelengths are chosen from an emission spectra study of exhaust gases. Those wavelengths have to be very sensitive to the gas temperature variation. We chose the spectral range located between 4.17 and 4.20 µm for which it exists an important thermometric effect (Figure 2). Moreover, $CO_2$ is the only emitting component in this range.

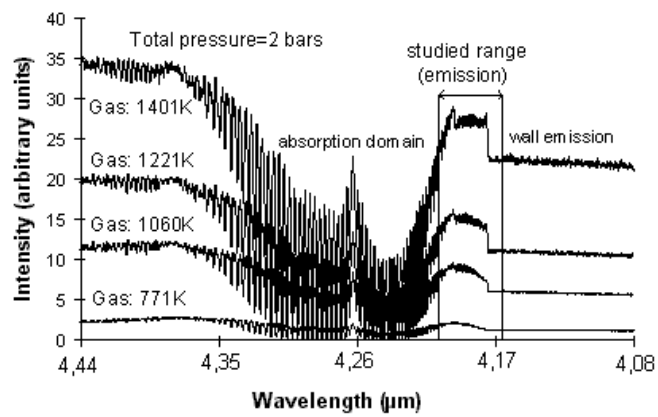



Figure 2: Influence of temperature on $CO_2$ emission spectrum

### Kernel specifics

An example of kernels for different wavelengths is given in Figure 3 for a temperature profile representative of exhaust gases. For the studied wavelengths, the kernels maxima take place at different abscises. An important feature is that none of the kernels have a significant value behind the hot point (highest temperature). In that region, it is then impossible to determine precisely which part of the gas corresponds to the main contribution of the measurement. Consequently, the

functions $(T,C)$ can not be accurately estimated behind a hot point. Moreover, as kernels partially overlap, measurements are correlated. A precise study of the condition number of the kernel correlation matrix shows that it doesn't exist more than 6 distinct informations in the studied spectral range.

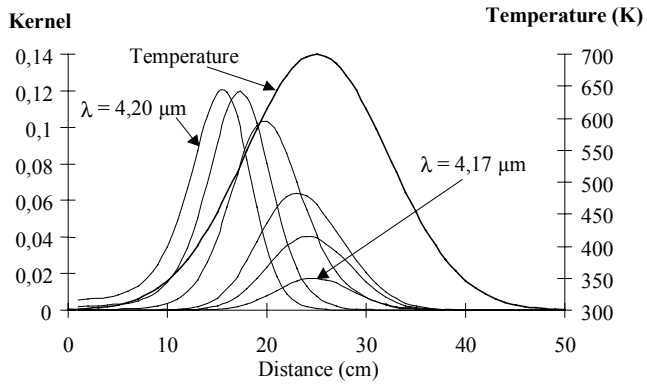
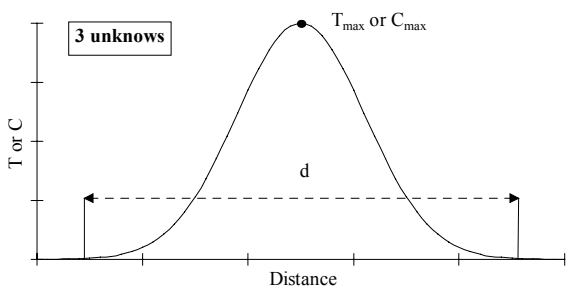



Figure 3: Example of kernels

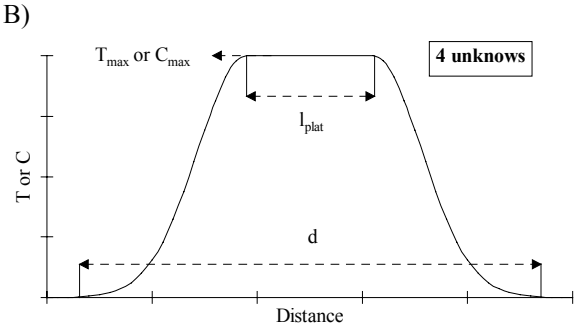
## Inversion algorithm

The study of the kernels shows that the number of distinct informations is less than 6. So in a first approach, we decrease the number of unknowns by using some a priori profiles representative of exhaust gases (Figure 4).

A) Gaussian distribution




B)




C)

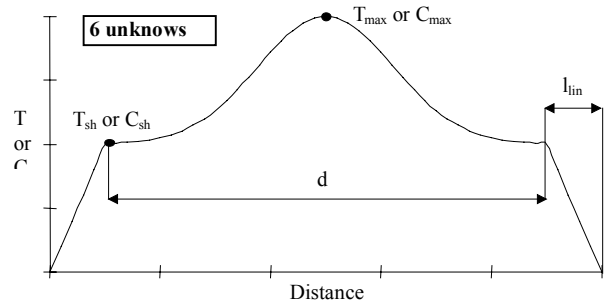



Figure 4: a priori profiles

The method was applied on a simulated experimental gaussian distribution with the above three a priori profiles. The quadratic criterion obtained for each case at the end of the inversion is given in Table 1.

Table 1: Results of inversion depending on the a priori profile

| a priori profile | Quadratic criterion |
|---|---|
| A) 3 unknowns | $1.5.\ 10^{-17}$ |
| B) 4 unknowns | $3.8.10^{-4}$ |
| C) 6 unknowns | $8.5.10^{-4}$ |
| D) Constant profile | 0.78 |

The minimum value of the final criterion actually corresponds to the solution. Yet, the measurement noise was not taken into account in these simulations.

Moreover, in order to improve the inversion convergence, some constraints on solution space are included. The physical limits of the unknowns $(T,C)$ are for exhaust gases:

$$280\ K < T < 1000\ K$$
$$330\ ppm < C < 10\%$$
Eq. (3)

For the axis problem, the quadratic criterion is given by:

$$J(T,C) = \sum_{n=1}^{N_\lambda} \left[L_{simul}(\lambda_n, T, C) - L_{meas}(\lambda_n)\right]^2 \qquad \text{Eq. (4)}$$

The criterion minimization is carried out with the Simplex non-linear algorithm. This method has the advantage not to use the criterion derivative. In our case, this derivative can not be analytically determined and the use of numerical derivative can trigger for the algorithm robustness.

By using the developed algorithm, some tests concerning the uniqueness result and the noise robustness of the inversion algorithm are carried out. The uniqueness is verified by

inverting a simulated spectrum with several initializations. The inversion results do not depend on those initializations and they correspond to the simulated functions. So, the solution is unique. To quantify the measurement noise effect on inversion results, we use a Monte-Carlo method. The inversion process is carried out N times with N different noises. This inversion repetition permits to determine the error induced by the noise on the functions $(T,C)$. For a signal to noise ratio equal to 7 (unfavorable case), we obtain an error of 0.5% on temperature and 7% on concentration.

The developed inversion algorithm is thus robust to inverse some real measurements with a good enough accuracy.

### Some examples of inversion results

Some radiation measurements were carried out in DeRA (GB) on exhaust gases of a SPEY engine (Rolls-Royce). This test setup has its own measurement system to determine gas temperature and $CO_2$ concentration. These measurements are based on an intrusive principle. In Figure 5, we compare these intrusive measurements to the inversion results of our optical measurements. The results show a good enough agreement between the two measurement methods although they are based on very different physical principles.

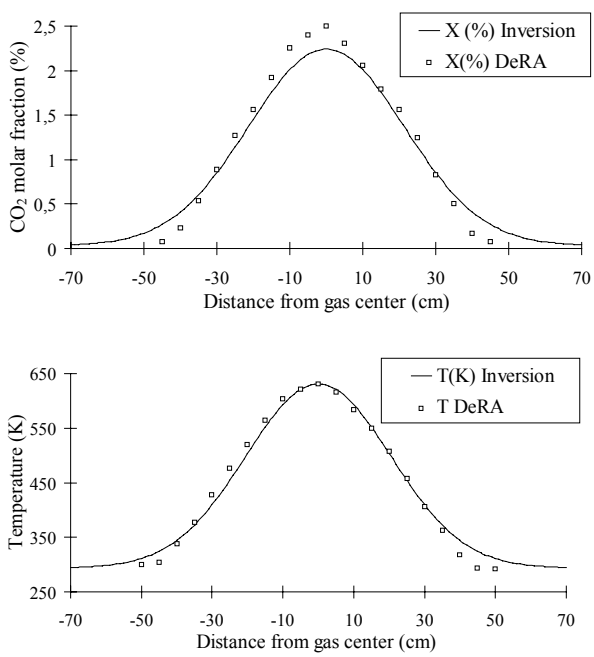



Figure 5: Comparison of results obtained with the intrusive and non-intrusive methods

## 3. TWO DIMENSIONAL INVERSE PROBLEM

In cases where the temperature or concentration distributions are not symmetrical, as at a cross section of a ramjet, we need to measure spectral intensities on the edges of a grid in X and Y directions (Figure 6). In the represented mesh, $N = N_1 + N_2 = 2\times 6$ measurements are made, $N_1 = 6$ on the X direction of the jet and $N_2 = 6$ on the Y direction. This is repeated for a set of $N_\lambda$ wavelengths [4]

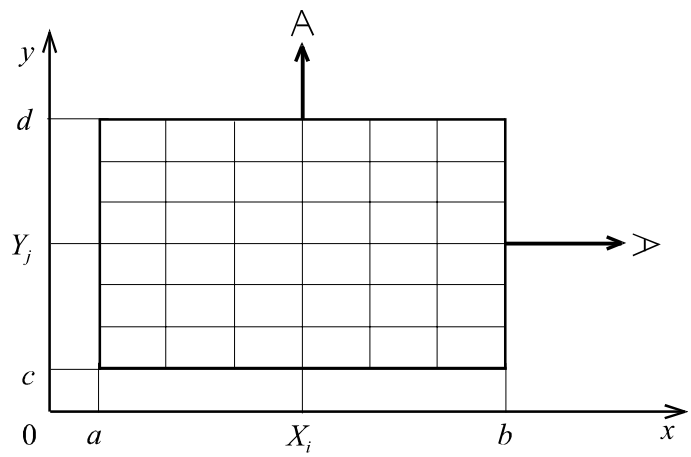



Figure 6: Diagram of the flame

The $N_1 N_2$ temperatures and the $N_1 N_2$ concentrations on the elements of the mesh are obtained from these measurements, associated with physical data and an adapted inversion algorithm.

Table 2: unknowns and measurements carried out in a 2D asymmetrical problem

| | |
|---|---|
| Number of unknowns | $2N_1N_2$ ( $N_1N_2$ temperatures, $N_1N_2$ concentrations) |
| Number of measurements | $N_\lambda(N-1)$ N measurements, the $N^{th}$ is a linear combination of the others |
| Physical data | Emissivity of one chosen component as a function of the temperature and wavelength |
| System to solve | $N_\lambda(N-1)$ non linear Fredholm equations of first type |

## Inverse problem

The equations of radiation transfer in a semitransparent medium are written for both directions of the grid, in the same form than in the axis problem. The equations give for each column or line, the theoretical expression of the spectral intensity transmitted by the semitransparent medium.

$$\int_a^b L^0(\lambda_n, T(X_i, y)) \frac{\partial \tau(\lambda_n, T(X_i, y), C(X_i, y))}{\partial x} dx = L_{meas}(Y_i, \lambda_n) \qquad \text{Eq. (5)}$$

$$\int_c^d L^0(\lambda_n, T(x, Y_j)) \frac{\partial \tau(\lambda_n, T(Y_j, y), C(Y_j, y))}{\partial y} dy = L_{meas}(X_j, \lambda_n) \qquad \text{Eq. (6)}$$

with $i = 1,2,..., N_1$, $j = 1,2,..., N_2$, $n = 1,2,..., N_\lambda$,
where:
$L^0(\lambda_n, T(x, y))$ is the Planck function,
$\tau(\lambda_n, T(x, y), C(x, y))$ is the transmissivity of the analyzed component,
$N_1, N_2$ are the numbers of measurements for each wavelength.

## Physical data

The main component produced by the hydrogen-air ramjet, $H_2O$, is analyzed. The $N_\lambda$ wavelengths chosen correspond to a domain where $H_2O$ is the single visible component. Three spectral ranges were selected among the emission bands of the spectra of water:

0.71-0.75µm, 1.78-1.88µm and 5-5.15µm

For each wavelength, intensity functions are highly sensitive either to the temperature or to the concentration. The theoretical intensities of a given molecule are obtained at different values of temperature with a model [5]. The results are validated for a fixed volume of gas (1 cm thick) and for a given concentration of the water (46%).

## Numerical algorithm [6], [7] .

To estimate $(T, C)$ distributions, the problem is to inverse the system of non-linear Fredholm-type equations, (5) and (6). The method that is proposed here is different of the one used for 1D problem.

The unknown functions are searched in the form of a combination of 2D-cubic B-splines. Therefore, the unknowns are the coefficient of the decomposition, called the approximation parameters.

The equations (7) and (8) give this decomposition on the 2D B-spline, produce of the 1D functions:

$$T(x, y) = \sum_{m=1}^{M_1^{(1)}} \sum_{k=1}^{M_2^{(1)}} p_{m,k}^{(1)} \varphi_m^{(1)}(x) \psi_k^{(1)}(y) \qquad \text{Eq. (7)}$$

$$C(x, y) = \sum_{m=1}^{M_1^{(2)}} \sum_{k=1}^{M_2^{(2)}} p_{m,k}^{(2)} \varphi_m^{(2)}(x) \psi_k^{(2)}(y) \qquad \text{Eq. (8)}$$

where:
$M_1^{(j)}, M_2^{(j)}$ are the numbers of approximation parameters, j=1 for the temperature and j=2 for the concentration,
$\left[p^{(1)}, p^{(2)}\right]^T$ is the vector of approximation parameters which dimension $\sum_{j=1}^{2} M_1^{(j)} M_2^{(j)}$ is fixed a priori.
$\left[\varphi^{(1)}, \varphi^{(2)}\right]^T$, $\left[\psi^{(1)}, \psi^{(2)}\right]^T$ are the one dimensional B-spline functions, in the domain [a,b]×[c,d].

To estimate these parameters, we use a minimization procedure of the residual functional J(T,C) by gradient methods:

$$J(T, C) = \frac{1}{2} \sum_{i=1}^{N_1} \sum_{n=1}^{N_\lambda} \left[F(X_i, \lambda_n, T, C) - L_{meas}(X_i, \lambda_n, )\right]^2 + \frac{1}{2} \sum_{j=1}^{N_2} \sum_{n=1}^{N_\lambda} \left[H(Y_j, \lambda_n, T, C) - L_{meas}(Y_j, \lambda_n)\right]^2 \qquad \text{Eq.(9)}$$

where F and H are the intensities computed from the radiative heat transfer equations (5) and (6) with the radiative properties of the chosen molecule.

The modified unconstrained conjugate gradient method is used. As the unknowns functions are parameterized (Equations (7)and (8)), the residual functional is a function of the approximation parameters $\left[p^{(1)}, p^{(2)}\right]^T$. At each iteration, the approximation parameters are improved as follows:

$$p_{m,k}^{(j),s+1} = p_{m,k}^{(j),s} + \gamma_j^s d_{m,k}^{(j),s} \qquad \text{Eq. (10)}$$

( $s$ is the iteration number)

The computation of the descent direction $\left[d^{(1)}, d^{(2)}\right]^T$ is made at each iteration from the calculation of the gradient of the $\left[g_1, g_2\right]^T$:

$$d_j^s = -g_j^s + \beta_j^s d_j^{s-1} \qquad \text{Eq. (11)}$$

with the coefficient $\beta_j^s = \dfrac{\left(g_j^s, g_j^s - g_j^{s-1}\right)}{\left\|g_j^s\right\|^2}$ and $\beta_j^o = 0$

The descent parameters $\gamma = \left[\gamma_1, \gamma_2\right]^T$ are computed using the linear estimation. They are obtained analytically by calculating the value that gives the highest increment of the residual functional between two iterations:

$$\Delta J^s = J^{s+1} - J^s$$

Their calculation thus necessitates to compute the derivative of $\Delta J^s$ towards $\gamma_1$ and $\gamma_2$.

The stopping criterion is obtained by the iterative regularization method [6]. This method is very successful in giving stable solutions of ill-posed inverse problem.
After each iteration, the convergence of the approximation parameters is checked:

$$\left|\frac{p_{m,k}^{s+1} - p_{m,k}^s}{p_{m,k}^s}\right| \le \varepsilon \qquad \text{Eq. (12)}$$

characterizing the sensitivity of the B-spline coefficient on the value of the temperature or concentration. $\varepsilon$ is a fixed small number.

In such minimization procedure, it is then necessary to compute the gradient $\left[g_1^s, g_2^s\right]^T$ at each iteration. By using the parametric form of the unknown functions (equations (7) and (8)), the gradient component is written as:

$$J_j' = G^{(j)} g_j \qquad \text{j=1,2}$$

where $G^{(j)}$ is the Gram's matrix for the basis functions.

$$G^{(j)} = \left\{ \begin{array}{l} G_{m,k,r,q}^{(j)} = \int_a^b \int_c^d \varphi_m^{(j)}(x)\psi_k^{(j)}(y)\varphi_r^{(j)}(x)\psi_q^{(j)}(y)\,dx\,dy \\ m = 1,....M_1^{(j)}; k = 1,....M_2^{(j)}; \\ r = 1,....M_1^{(j)}; q = 1,....M_2^{(j)}; j = 1,2 \end{array} \right\}$$

The gradient is then obtained by Cholesky decomposition, which is very stable numerically.

The calculation stops with the value of the residual criterion reaching the total measurement error:

$$J(T,C) \approx \delta^2 \qquad \text{Eq. (13)}$$

where:

$$\delta^2 = \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} \sum_{n=1}^{N_\lambda} \sigma_{ijn}^2$$

and $\sigma_{ijn}^2$ an estimate of the discrete error.

## Results

Tests of the procedure were made with simulated experimental measurements: constant and parabolic temperature and concentration fields. For the first one, the simulated fields were T=1500K and C=0.5%. The fields obtained after 126 steps are shown in Figure 7. To test the influence of errors possibly contained in measurements, a 10% perturbation introduced in the simulated measurements has led to a variation of concentration of 5% and a neglected variation of temperature. The second one showed a good agreement at the center of the domain but a worse one on the boundaries, in the area where transmission is close to the maximum.

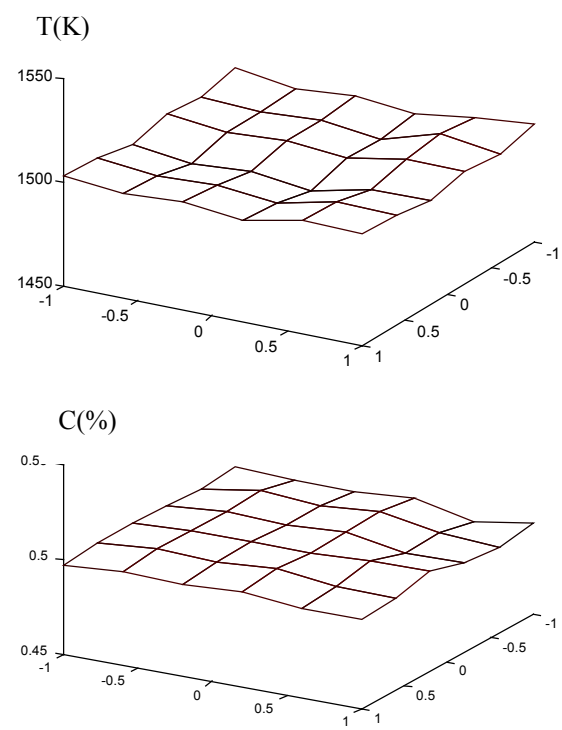



Figure 7: Temperature and concentration of $H_2O$ obtained from a simulated measurement of a constant field **(T=1500K and C=0.5%)**

Further validation is now needed with experimental data, including noise and error measurements.

## 4. CONCLUSION AND FURTHER PROSPECTS

Two inversion methods to determine one or two-dimensional temperature and concentration distributions in hot combustion gases were presented. For the 1D solution, given the analysis of experimental and physical data, a first approach using a priori profile is developed and gives satisfactory results. The 2D solution was validated on simulated experimental $(T,C)$ fields and showed a good agreement at the center of the domain. In future prospect, we want:

- to reduce the a priori information in the resolution of the 1D problem,
- to carry out an experimental device in order to test 2D resolution on real case,
- to improve the accuracy of the solution at the boundaries.

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## KEY WORDS

Spectroscopy, optimization, B-spline, iterative regularization