Chemical Species Tomography from Spectral Optical Attenuation Data

N. Polydorides[1*] and H. McCann[1]

[1] School of Engineering, Institute for Digital Communications, University of Edinburgh, Edinburgh, UK

[*]Email: n.polydorides@ed.ac.uk

ABSTRACT

We introduce a novel approach that casts a linear inverse problem for species concentration tomography from spectral data such as those acquired in wavelength modulation spectroscopy or direct absorption spectroscopy. Under isobaric measurement conditions and known plume temperature, our technique leads to a linear well-posed estimation problem for an extended data set derived from the direct absorption spectroscopy measurements. This allows imaging the concentration with enhanced noise robustness and spatial resolution that is significantly higher compared to previous methods for the same number of optical paths. We demonstrate the performance of our approach through proof-of-concept simulation for a carbon dioxide tomographic measurement.

Keywords Carbon dioxide concentration, chemical species tomography, linear attenuation.

Industrial Application Tomography of gases, emissions.

1 INTRODUCTION

Optical diagnostics are increasingly employed to image combustion and gas plumes, enabled by advances in opto-electronic components and image processing algorithms. Chemical species tomography (CST) is one such tool, which reconstructs the distribution of scalar properties of a gas from measurements of light made at the periphery of the flow domain. For a recent topical review of methods and applications we refer the reader to Cai and Kaminski (2017). CST was initially developed to infer the concentration of an absorbing gas under isothermal, isobaric conditions using measurements of monochromatic light absorbance. Since the advent of tunable laser signals, the technique has been extended to include the simultaneous estimation of temperature and concentration. Multi-parameter estimation can be achieved by considering a non-linear inverse problem, in which the temperature and concentration of a target species are inferred from multispectral absorption data by a combined model of radiative transfer and line-by-line spectroscopy. In principle, such an approach can lead to the reconstruction of the absorbance spectrum over a range of wavenumbers, from where temperature and concentration can be estimated locally, by solving an ill-posed inverse problem by following a Bayesian estimation algorithm or an optimization as explained in Daun et al. (2016) and Polydorides et al. (2016) respectively.

1.1 Governing spectroscopic models

We begin to describe our methodology by presenting the model equations for simulating the direct absorption spectroscopy (DAS) measurements, here assumed taken on a single chemical species such as for example carbon dioxide. Given spectroscopic information from the HITRAN database by Gordon et al (2017), and considering spatially varying profiles of plume temperature and concentration, in isobaric condition the absorbance spectrum from a single optical axis L is ideally modelled as documented in Hanson et al. (2016)

$$\alpha(\nu) = \sum_{j=1}^{N} \int_L \ dx\, S_{\nu_j}(T)\phi_{\nu_j}(T,P,X) P\, X \tag{1}$$

where the sum runs over the N HITRAN spectroscopy lines. In the above expression, T is the temperature, P stands for pressure and X is the targeted species' molar fraction. Note that T, P and X

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enter the definition of the line shape functions ϕ_{ν_j}while the line strength functions depend exclusively on the temperature. Introducing the kernel function

$$W_{\nu_j}(x,\nu) = S_{\nu_j}(x)\phi_{\nu_j}(x,\nu) \tag{2}$$

With x and ν the spatial and spectral coordinates respectively, allows to cast the DAS measurement model at ν as a nonlinear integral equation

$$\alpha(\nu) = \sum_{j=1}^{N} \int_L \ dx\, W_{\nu_j}(x,\nu) P\, X \tag{3}$$

Typically, one measures the spectral absorbance $\alpha_{\text{meas}} = \{\alpha(\nu_1), \ldots, \alpha(\nu_k)\}$ at k wave numbers at the characteristic range of the targeted species, on each beam intersecting the plume. Thereafter, these data are usually processed by means of regression to yield, in the knowledge of T and P, the line integrals

$$C = \int_L \ dx\, X \tag{4}$$

When calculated on a sufficient number of beams, C allow to estimate quantitatively the profile of X using conventional tomographic algorithms such as Radon transform inversion or regularised algebraic reconstruction methods. However, due to the intrinsic complexities of the in-situ measurements in harsh environments, the CST problems tend to be severely under-determined, leading to limited-data and sparse tomography applications, see for example Terzija et al. (2011) and Polydorides et al. (2016). In this work we demonstrate, by means of simulation, an alternative strategy where the nonlinear model (3) is linearized to form an alternative model for X, using directly the spectral data. In effect, this leads to having more linearly independent data for reconstructing X and thus allows to utilise a least squares formulation with a minimum amount of regularisation.

1.2 Inverse problem

Our approach to the image reconstruction inverse problem exploits the weak dependence of the lineshape function on the targeted concentration. In fact, when knowing an average value of the molar fraction $\bar{X}$, for a constant pressure P we can approximate

$$\frac{\alpha(\nu)}{P} = \int dx \ W_{\nu_j}(x,\nu;X,T)X(x) \approx \int dx \ W_{\nu_j}(x,\nu;\bar{X},T)X(x). \tag{5}$$

Discretising on a finite dimensional grid with n elements, the DAS model for the measurement at ν becomes

$$\frac{\alpha(\nu)}{P} = \ell_j \operatorname{diag}\left(w_{\nu_j}\right) X. \tag{6}$$

where ℓ_j is the discretised line integral operator along the jth optical trajectory, the vector w_{ν_j} has entries

$$w_{\nu_j} = \sum_{j=1}^{N} W_{\nu_j}(x,\nu;\bar{X},T) \tag{7}$$

and X is the discretised sought concentration vector. Populating the above for k different wave numbers yields a system for the spectral measurements α_{meas} as

$$P^{-1}\alpha_{\text{meas}} = W^T \operatorname{diag}(\ell_j) X \tag{8}$$

While applying the same model for all m optical paths in the measurement system we eventually arrive at

$$\alpha = BX = \begin{pmatrix} B_1 \\ \ldots \\ B_m \end{pmatrix} X \text{ , where } B_j = PW^T \operatorname{diag}(\ell_j) \tag{9}$$

is $k \times n$ and B is $mk{\times}n$. Note that contrary to the conventional approach in (4) we now have substantially more equations for the same unknown. To be precise the number of equations we get from this model is equal to the numerical rank of the matrix B, which in turn depends on that of $W$and the sum of the vectors w_{ν_j}. It can be shown that if T is not constant over the field of view then the rank of B is much greater than m. Thus upon choosing the grid dimension appropriately the image of X can be traced iteratively, beginning with $\bar{X}$ by solving an unregularized least squares problem. We find that this result is exceptionally useful, as it takes advantage of the richness of the spectral information and at the same time it alleviates the need for regularisation.

1.3 Numerical example

We demonstrate the proposed method by means of a simulated example. Assuming the FLITES measurement system described in Polydorides et al. (2016) and Polydorides et al. (2018) which consists of 126 straight optical beams from 6 projection angles and we discretise the domain into a 30 x 30 square pixels grid. Notice that in the conventional approach one has a heavily underdetermined problem with 126 data points and 900 unknowns. Moreover we assume inhomogeneous concentration and temperature profiles as shown in figure 1, at a constant pressure of 1.5 atm. In this setup we take 500 spectral absorbance measurements on wave numbers equally spaced between 5005 cm^{-1} and 5008 cm^{-1}, as shown in figure 2, based on 34 HITRAN spectroscopy lines.

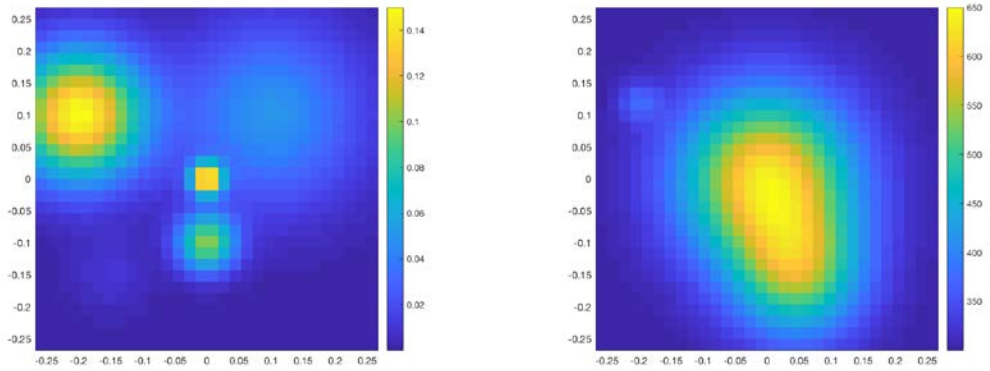

Figure 1. Left, the targeted CO_2 concentration profile and right the temperature distribution over the same area.

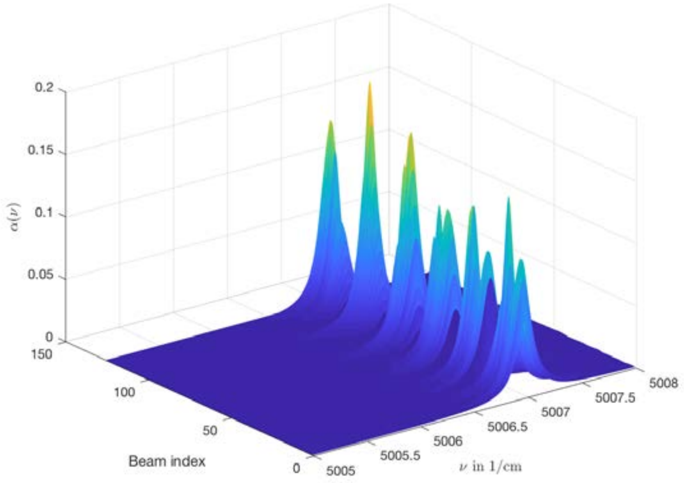

Figure 2. The spectral absorbance DAS measurements on 126 optical channels corresponding to the concentration and temperature profiles shown in figure 1.

In these circumstances, the matrix B has dimensions 63000×900, while the unknown vector X also has dimension 900. For a small level of synthetic noise in this data we solve the least square problem for an initial guess $\bar{X}=0.027$, leading to a matrix B with rank 881 and a first iteration image shown to the left of figure 3 with relative error of 4.5%. Reiterating based on this estimate for the concentration yields a full rank matrix B and a 0.0008% relative error, as it is evident from the resemblance of the image in the right of the figure 3 to the original target shown in figure 1.

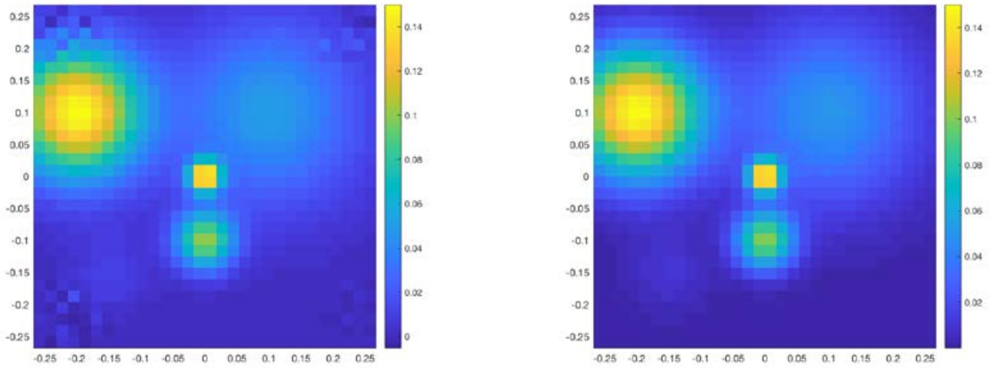

Figure 3. The first and second iterations of the image reconstruction without any regularisation. The one to the left is based on an initial homogeneous guess of the concentration and the one to the right uses the one to the left as an initial guess.

1.4 Conclusions

In this short paper we outlined a new approach which leads to posing a linear inverse problem for the concentration of a chemical species directly on direct spectroscopy data without the need to resolve path concentration integrals beforehand. Using numerical simulation, we have showed that when the temperature profile of the plume is inhomogeneous it is possible to deduce a large number of linearly independent equations for the concentration even from a small number of optical channels. In turn, this implies that in knowing the temperature of the plume we can image its concentration with higher spatial resolution.

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