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SYNOPSIS: As it is well known in algebra, it is always possible to cancel a vector by taking its inner product with an other vector which is orthogonal to it. A method based on this concept enables one to construct a spectrum, which we have called adjoint spectrum, that has the power of annihilating an undesired interference spectrum. This makes the monitoring of a specific atmospheric gas by spectrometric methods impermeable to interferences. Mathematical descriptions will be made of the notion of the adjoint spectrum, numerical examples and experimental results confirming the effectiveness of the so called spectrum when applied to the resonance absorption method will be reported as well.

1. INTRODUCTION

Many spectrometric techniques of measuring very low concentrations of air pollutants with a high precision have been reported[1,2]. However, they failed far from reaching the theoretical detection limit given by the detector noise because of the vulnerability of spectrometers to various interferences[3]. This paper deals with a method to design a numerical filter that has the power of annihilating designated

interference spectra. The mathematical foundation is explained, and numerical examples as well as experimental results prooving the noise rejection effects of our technique are also reported.

2. Mathematical concept of adjoint spectrum

Let Sr a known spectrum (reference spectrum) of the gas species considered. In the absence of any interference, a spectrum Sxo relative to the same gas species in the atmosphere can be expressed as

$$Sxo = k Sr$$
 (1)

where k is a constant, the knowledge of which gives the desired value of the gas concentration. However, what we really measure is a spectrum Sx which includes a noise spectrum Sn that results from various types of interferences, as illustrated in Fig.1, which is expressed in this case as,

$$Sx = k Sr + Sn$$
(2)

If now we can choose a spectrum $\boldsymbol{S}^{\boldsymbol{\star}}$ that satisfies the following two conditions

$$= 0$$
 (3)
and $= 1$ (4)

then k will be determined by taking the inner product of S^{\star} with both sides of eq.(2) as



Fig.1 Illustration of an adjoint spectrum.

 $<S^{*},Sx> = k$ (5)

 S^* is then the desired adjoint spectrum.

The geometrical illustration of Fig.1 shows that the spectrum obtained by projection of Sr on the direction perpendicular to Sn when devided by the square of its length satisfies both conditions of an adjoint spectrum,

$$S^* = P_{Sn}(Sr) / ||P_{Sn}(Sr)||^2$$
 (6)

where P stands for projection.

If now we define a linear subspace T of dimension I that is spanned by all the interference spectra involved, $T = \{Si, i=1, 2, ..., I\}$, then an orthonormal base {Ui, i=1, 2, ..., I} can be established as

$$U_{i} = \frac{(S_{i} - \langle S_{i}, U_{j} \rangle U_{j})}{\|S_{i} - \langle S_{i}, U_{j} \rangle U_{j}\|}$$
(7)

as a result, the adjoint spectrum as defined by eq.(6) can be deduced by

$$S^{*} = \frac{(S_{r} - \langle S_{r}, U_{i} \rangle U_{i})}{\|S_{r} - \langle S_{r}, U_{i} \rangle U_{i}\|^{2}}$$
(8)

3. Application of the adjoint spectrum

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3.1 Theoretical example

As illustrated by Fig.2, the upper trace of (d) shows a spectrum Sx that is a linear combination of a reference spectrum Sr (b) and 3 representatives of noise spectra (1), (2), and (3) in (a). The lower trace of (d)is the desired pure spectrum obtained after annihilation of noise by applying the adjoint spectrum S* in (c) to Sx.

3.2 Practical situation

The practical situation is quite different from that of the ideal case considered above in that, neither the reference spectrum nor the interference spectra are known precisely. Therefore the crucial problems we have to overcome for a maximum effectiveness of the adjoint spectrum are: (1)how to get a pure reference spectrum? and (2) what kind of interferences should be involved in the noise process and to what degree they affect the results?. If one can get a nearly pure reference spectrum with an appropriate optical system and through synthesizing of low pressure spectra, it is not the case for interference spectra. However, while systematic interferences can be more or less precisely known through transform techniques, i.e.Fourier transforms, others can only be approximated by statistical methods. One important feature of the adjoint spectrum that helps dealing with this problem is that it acts only on the designated interferences without affecting the desired signal. This provides to some extent a large degree of freedom in choosing the interference spectra. In other words, even if the expected noise spectrum does not really exist, this will affect only slightly the results. However, it is still necessary to define the security limits relative to a certain practical situation within which one can apply the adjoint spectrum technique. This will determine particularly the maximum number of the expected interference spectra may allow to achieve the minimum that one error in the value of the measured gas density.



(c) Adjoint Spectrum

Fig.2 Numerical example of an adjoint spectrum.



Fig.3 Application of the adjoint spectrum to a Pb-TDLAS

3.3 Experimental results with a Pb-TDLAS system

Fig.3 illustrates clearly the effect of the adjoint spectrum when applied to a Pbsalt TDLAS. A temporal atmospheric methane density is shown in (a) where an adjoint spectrum is used to reduce only a flat baseline error. While (b) is the temporal trace of the same gas when an adjoint spectrum is involved that takes account of more types of interferences.

4. Conclusion

We have explained in this report about a notion of adjoint spectrum that has the power of annihilating noise spectra in spectrometric measurements, theoretical examples have been given and experimental results with a Pb-TDLAS have been reported as well.

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