SATELLITE MEASUREMENTS OF TRACE GASES USING BLIND SOURCE SEPARATION

Pia Addabbo, Maurizio di Bisceglie

Università degli Studi del Sannio
Piazza Roma 21, I-82100, Benevento, Italy
pia_addabbo@yahoo.it, dibisceg@unisannio.it

Abstract

Two algorithms are currently adopted for producing accurate measurements of trace gases from satellite data: the Band Residual Difference (BRD) algorithm [1] and the Linear Fit (LF) algorithm [2]. The BRD is based on the evaluation of differential residuals due to the trace gas at several wavelength pairs; spectral bands are selected where large absorption peaks are displayed to improve the algorithm accuracy and discrimination from other gases [3]. The linear fit algorithm is based on fitting a linearized radiative transfer model plus a loworder polynomial to the logarithm of the reflectance spectrum. The methods are physically grounded and, at the current stage, they are able to measure gas concentrations with a good level of accuracy. Possible improvements could be expected by fitting a wider portion of the observed spectrum and by fully (spectral) exploitation of the gas absorption spectra.

We propose here a new method where the joint use of canonical measurements and statistical concepts is used to exploit the whole UV spectral band. We assume that the overall absorption from the atmosphere is due to statistically independent contributions; this is the main constraint to approach separation of the single spectra using a technique referred to as Independent Component Analysis (ICA) or Blind Source Separation. From m Instantaneous Field Of Views (IFOV) m spectra $[x_1(\lambda), x_2(\lambda), ..., x_m(\lambda)]$, with λ the wavelength, are observed. They represent the linear combination (or mixing) of n unknown components $[s_1(\lambda), s_2(\lambda), ..., s_n(\lambda)]$, with $n \leq m$, that are assumed to be mutually statistically independent. This is physically grounded when statistical spectral dependencies due to chemical and physical gas interactions can be neglected. We let $\mathbf{x}$ the vector of observations and $\mathbf{s}$ the vector of independent components so we may write, using matrix notation, $\mathbf{x} = \mathbf{As}$. Here, $\mathbf{A}$ is the unknown $m \times n$ mixing matrix. If we invert this equation, we obtain $\mathbf{s} = \mathbf{A}^{-1}\mathbf{x}$, so, the basic problem is to estimate $\mathbf{A}^{-1}$. In the absence of additional information about the single waveforms, the standard ICA works by maximizing the statistical independence of the components of $\mathbf{s}$. This task is usually carried out by ad-hoc algorithms based on maximization of the Mutual Information, such as RADICAL (Robust Accurate Direct ICA aLgorithm) or FastICA.

This is, however, a simplified situation since we are not really concerned with a standard signal separation problem where the number of component is exactly known. On the contrary, a nonzero trace gas concentration can be present only in some fields of view. This poses, in general, an additional detection problem embedded in the estimation procedure. To overcome this difficulty we have introduced a known contamination in the IFOV under test, obtained by adding an attenuated version of the reference spectra to be investigated. This artifice provides two favourable effects: a) it prevents unreliable results when the waveform is actually absent, b) it acts by driving the solution towards a known set of waveforms when they are actually present.

The procedure, that we state for simplicity for two components, is summarized hereafter

1. for each IFOV two observations are defined as follows:
   (a) the reflectance spectrum $x_1(\lambda)$ in a range of wavelengths (λ_1, λ_2);
   (b) a contaminated spectrum $x_2(\lambda)$ in the same range of wavelengths generated by injecting a small contribution from a reference spectrum;
2. the mixing matrix is estimated by maximizing independence between spectra.
3. the spectral waveforms $[s_1(\lambda), s_2(\lambda)]$ are retrieved through matrix inversion. The matrix coefficients are also used for evaluating gas concentrations.

The ability of the algorithm to separate different reflectance spectra has been investigated with reference to SO_2 retrieval from the Ozone Monitoring Instrument (OMI) on board Aura platform. The reflectance spectra, in the range 270–330 nm, have

been evaluated from the interpolated radiance spectra normalized to the (daily) sun irradiance spectra and the absorption cross spectrum of SO_2 has been used as a reference for contamination.
Results obtained after processing the data acquired during the eruption of Anatahan volcano on April 06, 2005 are shown in (figure 1) (left hand side). To plot the images, we have evaluated the energy of the SO_2 reflectance spectrum retrieved from any IFOV. The center figure shows the corresponding image for Planetary Boundary Layer (PBL) SO_2 column (OMSO2 dataset, available from Goddard Earth sciences Data and Information Services Center, produced with the BRD algorithm). A truecolour image from Aqua-MODIS pass (April 06, 2005) is also shown. Aqua orbit is 15 minutes before Aura orbit.

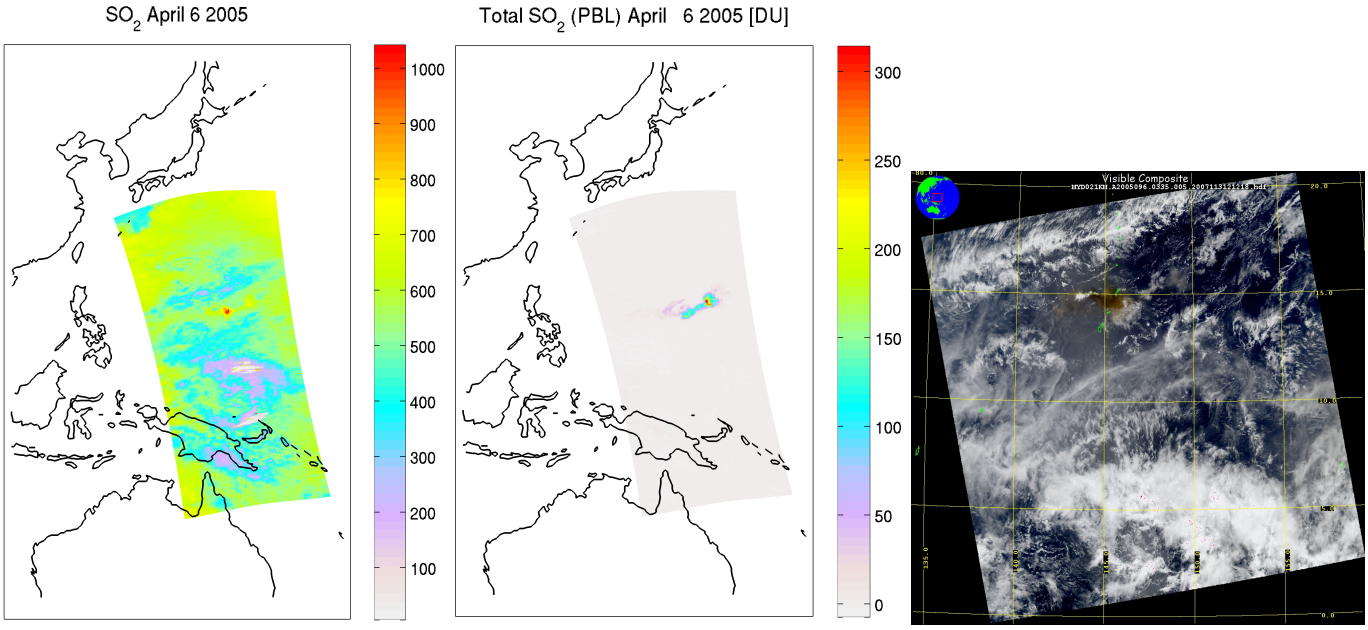

Fig. 1. SO_2 concentration from Anatahan volcano eruption (April 06, 2005) using: Left) Blind Source Separation, Center) BRD algorithm. Right) Modis–Aqua Truecolor image, (April 06, 2005).

By comparison between the Blind Source Separation and BRD algorithms, it is apparent that the SO_2 cloud is correctly detected in both cases. It is also evident that cloud artifacts are not removed in the BSS algorithm and that higher values of SO_2 concentration are shifted to the right side in the left hand image with respect to the center image. The visual inspection of Modis–Aqua image shows, however, that the shape of the brown cloud is more significantly correlated to our case. The algorithm is in its first stage of creation and refinements are necessary in many contexts ranging from clouds correction to calibration of the SO_2 concentration in Dobson units. On the other hand, results seem to be promising, also in view of retrievals of different atmospheric components.

References

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