Dedicated Neural Networks Algorithms for Direct Estimation of Tropospheric Ozone from Satellite Measurements

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Abstract—**In this paper we report on the design of a Neural Networks algorithm to retrieve tropospheric ozone information from satellite data. Following a combined radiative transfer model-extended pruning sensitivity analysis for input wavelengths selection, we first made an inversion exercise based on a synthetically produced radiance-tropospheric ozone concentrations database. Starting from the encouraging obtained results, we tested the Net on ESA-ENVISAT SCIAMACHY Level 1b data. A time series of Tropospheric Ozone Columns on some midlatitude sites has been retrieved from the satellite measurements and then compared with collocated and simultaneous ozonesondes reference columns. The inversion results are presented and critically discussed.**

I. Introduction

The ozone is an atmospheric constituent of a crucial importance for the life in Earth's biosphere, owing to its role in screening the harming UVB and UVA solar radiation. About 90% of atmospheric ozone is in the stratosphere where it carries out its work of absorbing UV radiation in Hartley and Huggins bands, contributing to the determination of the vertical temperature structure and dynamics of airmasses. The remaining 10% of atmospheric ozone is in the troposphere. Tropospheric ozone is a direct greenhouse gas [1]. In the last decades enhancements in anthropogenic emissions of photochemical ozone precursors in the lower troposphere may have changed the balance, leading to the increase of ozone concentration in troposphere; this enhancement has been estimated to provide, after carbon dioxide and methane, the third largest increase in direct radiative forcing since the pre-industrial era [1]. Besides the climatic effects, these enhancements can have as well dramatic effects on public health and on vegetal culture growth. A global and continuous monitoring of ozone levels in the troposphere is necessary. Ground-based and ozonesonde monitoring is mainly used for observing, studying and monitoring the ozone in troposphere; obviously these techniques cannot provide a global and continuous coverage. A suitable choice could be satellite monitoring; this technique, however, presents a number of problems in terms of spatial resolution and sensitivity to ozone in the lower layers of atmosphere. For these reasons the present satellite techniques of tropospheric ozone monitoring are based on effectively indirect retrieval methods such as Tropospheric Ozone Residual (TOR) method, see e.g. [2], or integration of the tropospheric ozone concentrations from pre-inferred ozone profiles, see e.g. [3].

We tried to circumvent these problems developing a direct methodology based on Neural Networks (NNs) algorithms which uses nadir measurements for the retrieval of information on ozone contents in troposphere, e.g. inferring the Tropospheric Ozone Column (TOC). In this paper we first present the results obtained by means of a sensitivity study performed with the LibRadtran suite [4]. The study aims at exploring the relative information budget in UV and VIS spectral ranges, in relation to tropospheric sounding. The satellite signal has been produced as to simulate ESA-ENVISAT SCIAMACHY data. Secondly we report on the performance of the subsequently designed Neural Network algorithms, specifically dedicated to tropospheric ozone retrievals from simulated ENVISAT-SCIAMACHY radiance spectra. In addition we present an inversion exercise based on real SCIAMACHY Level 1b data. NNs are composed of some computational elements called neurons, linked with weighted synapses. In the training phase, the NN learns the mapping between input and output vectors by optimizing the synapses' weights. It has been demonstrated that, providing that the learning dataset is representative of the phenomena to be modeled and a sufficient number of processing units is considered, NNs, in particular Multi Layer Perceptrons, can approximate any continuous mapping function with the desired accuracy. We thoroughly discuss the input wavelength selection and the optimization of the topology of the Nets. In particular for which concerns the selection of the inputs, we adopted a combined radiative model-NN extended pruning procedure.

II. The SCIAMACHY spectrometer

The SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY) instrument, onboard the ESA-Envisat spacecraft, is a nadir/limb/lunar and solar occultation viewing spectrometer that can operate in the UV/VIS/NIR range (214 to 2386 nm), with a spectral resolution of 0.24-1.48 nm (0.24-0.48 nm in our spectral region of interest) and a nadir spatial resolution of typically 30 km along track X 60 km across track [5]. The technical characteristics of the SCIAMACHY spectrometer are compatible with a good quality atmospheric monitoring.

III. Sensitivity study of a simulated satellite nadir UV/VIS radiance measurement to tropospheric ozone variations

The sensitivity of nadir satellite signals to tropospheric ozone concentrations and their changes is a topic of present research on air pollution monitoring from space. To investigate the possibilities and limits of inferring the tropospheric ozone variations from satellite data we analyzed the variations in Earth's radiance resulting from changes of ozone concentration at different tropospheric heights. At this stage we used the UVSPEC radiative transfer model and the LibRadtran libraries [4] to represent a summer midlatitude urban environment. The atmospheric state was set by choosing vertical profiles of air density, pressure and temperature, and ozone, oxygen, water vapor, carbon dioxide and nitrogen dioxide concentrations as in AFGL midlatitude summer climatological standard. The solar spectrum was chosen at a resolution of 0.05 nm (*ATLAS PLUS MODTRAN* spectrum) and then interpolated at the operating wavelength of SCIAMACHY sensor in the interval 220-800 nm. The solar zenith angle (sza) has been put at a fixed value of 30°, and observation geometry has been put as an exact nadir measurement (zenith and azimuth angles equal to 0). The SCIAMACHY sensor has been three fold modeled: a) the model was forced to solve the radiation transfer equation at the operating SCIAMACHY wavelengths, b) a Gaussian slit function with a FWHM = 0.3 nm was imposed to simulate the sensor's spectral resolution, and 3) a 1% level noise was added to the modeled radiances. Starting from these assumptions, the ozone concentrations were systematically enhanced at the tropospheric heights (0-14 km in our case) and the changes in backscattered UV/VIS spectra were analyzed. Figure 1 shows the differences of Earth's radiance in the spectral range 220-800 nm, for a doubling of ozone at four height levels with respect to standard case. The maximum sensitivity, for changes at all height levels, is in the range 302-307 nm, mainly due to total ozone variations. A little sensitivity is also reported in the VIS range (around the interval 550-650 nm, in the Chappuis bands). To test the overall tropospheric information budget, we performed an integration of the mentioned differences in the sensible UV and VIS intervals for enhancements at each height level, calculating some sort of UV and VIS radiative forcing at fixed observation angle. The trends of these quantities are reported in figures 2 and 3. Figure 2 shows also the fitting of UV forcing with three functions *F(z)*. The sigmoidal fitting function seems to approximate with a good accuracy the trend of these values. Although noticeable dispersion, VIS forcings, and consequently VIS tropospheric information budget, seem to be not negligible. Considering the observed large noise levels and the need of accurately knowing surface albedo values, this sensitivity in Chappuis ozone bands can be exploited, in combination with UV information, to retrieve

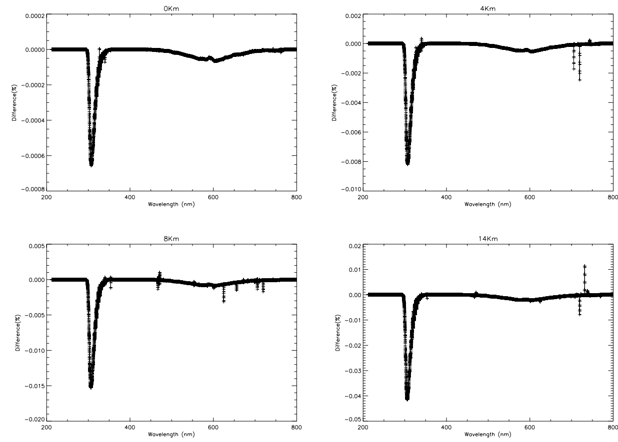

Fig. 1. Spectral differences between Earth's radiance in midlatitude standard atmospheric conditions and the standard case plus doubling at the height level z=0, 4, 8 and 14 Km.

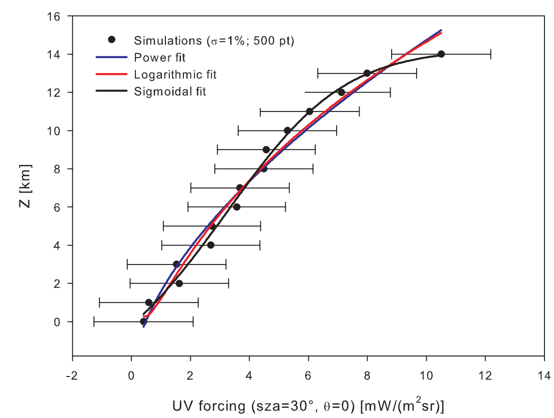

Fig. 2. Dependence of UV radiative forcing at fixed observation angle for ozone doubling, with height. Some fitting functions are also represented. For sigmoidal fit $R^2 = 0.99$.

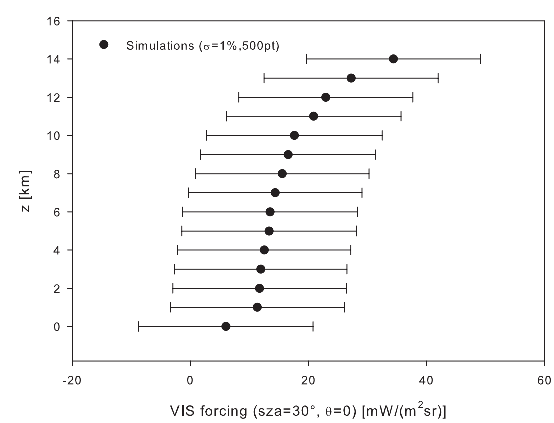

Fig. 3. Dependence of VIS radiative forcing at fixed observation angle for ozone doubling, with height.

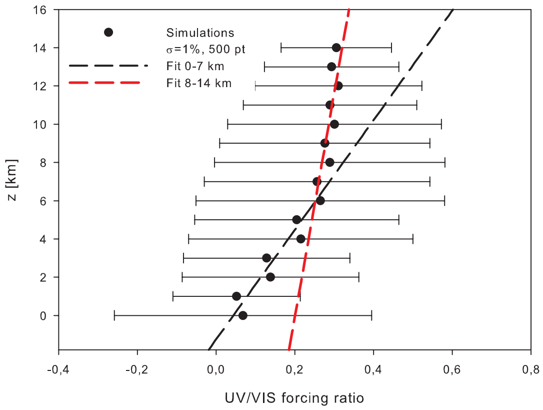

Fig. 4. Dependence of UV/VIS forcing ratio with height. Two different fitting functions for the two height ranges 0-7 km and 8-14 km are reported.

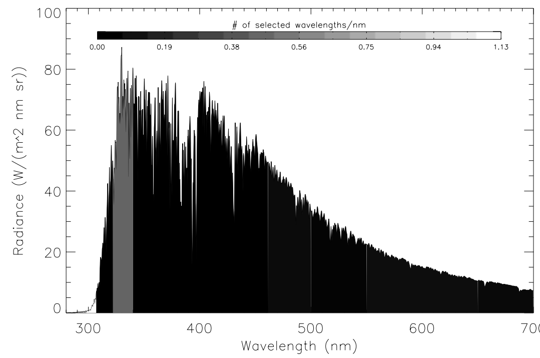

Fig. 5. Density of the selected wavelengths, in terms of number of selected wavelengths per nm, at the end of the pruning procedure

tropospheric ozone information from UV/VIS satellite data. An interesting parameter for our purposes is the ratio of the UV and VIS forcings above mentioned. In figure 4 the vertical trend of this quantity for our simulated data is depicted. Qualitatively the UV/VIS forcing ratio has a linear trend in the first height levels, and tend to saturate at a fixed value for z higher than 8 km. This behavior renders this parameter quite interesting for sounding the lower atmospheric heights, though uncertainties are large.

From this simple exercise is possible to notice that a) the retrieval of height resolved information on tropospheric ozone is quite difficult owing to the low sensitivity, especially in the lower height levels and the large theoretical standard deviations, and b) the VIS range can have an interesting role for this issue. NNs are particularly intended to work in cases of non-linear dependency between physical quantities. In some cases, weak dependencies can be found with the aid of NNs. From this point of view, this sensitivity analysis suggests a possible employment of such class of algorithms.

IV. NNs for TOC retrievals from modeled UV/VIS satellite data: design and preliminary results

A. Dataset preparation

Our first inversion exercise was referred to Tropospheric Ozone Column (TCO) retrieval; we plan to investigate the height resolved retrieval potentiality of our Nets in the future. Our first inversion exercise was referred to a synthetic database of input-output pairs. We generated 4000 ozone profiles and we calculated correspondingly the Earth's radiance as described in the previous section, by means of the UVSPEC model. The tropopause has been considered in the range 14-17 km. The total ozone was varied between 350 and 250 DU. For part of the profiles, an additional contribution modeled by an exponential function to simulate ground production of ozone and some vertical transport has been considered. It has to be noticed that this dataset preparation doesn't pretend to model specific pollution phenomena with accuracy but is intended only to provide an extended dataset to investigate the inversion potentiality of our NNs. The input wavelength selection and the results of this kind of exercise are proposed in sections IV-B and IV-C. We tried to use also measured radiances extracted from SCIAMACHY Level 1b data. Satellite data were matched with collocated ozonesondes measurements from WOUDC and SHADOZ databases, as in [7]. We considered only midlatitude sites. The results of this second exercise are proposed in section IV-D.

B. Extended pruning

For exploring the information budget of the SCIAMACHY UV/VIS bands, we performed an extended pruning (EP) procedure as described in [6], using the mentioned synthetic database of radiance-TOC pairs. We first selected the radiance data in the range 280-700 nm for the dataset described in section IV-A, and we matched the spectra with the profiles, correspondingly. For shortening the computational time we didn't consider radiance data in the regions where tropospheric ozone showed very weak sensitivity, following the indications of section III. The TOC were derived by means of the integration of ozone concentrations from 0 to 14 km. We first trained the Net for several hundreds of learning cycles. Then we started the pruning procedure by applying the following iterative steps:

- the weakest synapse is pruned;
- the net is re-trained without re-initialization;
- the error E is calculated and the pruning is stopped if $E > E_{\text{max}}$.

An input neuron is eliminated when all its connections are pruned. Figure 5 shows the density of the selected wavelengths after the whole procedure. Some interesting features clearly emerged. The input wavelengths in the region 307-322 nm are quickly pruned, and we can find a very little density even after reasonably few pruning steps. In general the higher density can be found in the range 298-307 nm and the relative importance of this band became more and more pronounced as the pruning went on; this band also showed the maximum sensitivity as showed in section III. The range 322-340 nm

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is second in importance; it has to be noticed that this band contained the whole required signal for the ESA-ERS2 GOME based NN described in [6]. In the VIS the density of selected wavelengths reflects the structure of Chappuis band and is in good agreement with VIS results of section III, with a maximum of information density in the band 550-650 nm.

C. UV/VIS NN inversion test with a synthetic database

Following the wavelength selection reported in section IV-B, we selected 28 UV/VIS input wavelengths. We considered also a hidden layer of 28 neurons. In [8] it was shown that the obtained NN showed an interesting retrieval capability, enhancing of over 10% the correlation coefficient of the retrieved and the test TOCs, with respect to UV-only case, on a test set of 1000 input-output pairs. In particular see figures 7 and 9 of the mentioned paper for details.

D. A test study at midlatitude: Uccle, Belgium, and Debilt, Nederlands stations.

Following the combined UVSPEC-EP sensitivity study of sections III and IV-B, and the inversion exercise with synthetically produced data of section IV-C, we tried to invert a set of real SCIAMACHY data. We considered the database described in section IV-A. We preprocessed and normalized the satellite data and we considered the integration of ozonesondes concentrations in the range 0-14 km as representative of the TOC at midlatitude locations. We obtained over 4000 input-output pairs. The topology of the considered Net is the one described in the previous section. We trained the Net with part of these data and we tested the results with an independent subset, considering a combination of Uccle, Belgium (50.8°N-4.4°E) and Debilt, the Nederlands (52.1°N-5.2°E) overpass data. The stations have been considered simultaneously because their distance is lower than the matching distance between satellite pixels' central coordinate and ozonesondes sites. It has to be considered that data from these two stations were not present in the training dataset. The time series of the NN TOC retrievals and reference ozonesondes TOCs in a time window of over a year is reported in figure 6. Though a systematic underestimation is clearly visible, it is possible to notice that the time trend is well reproduced from our Net's retrievals.

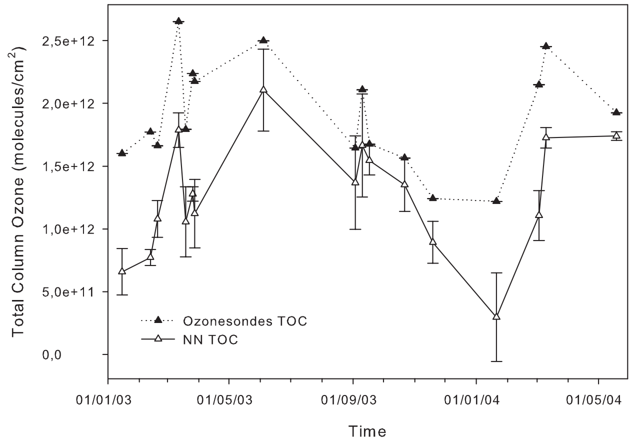

Fig. 6. Time series of the retrieved (open triangles with errorbars) and simultaneous reference ozonesondes TOCs (filled triangles) at Uccle and Debilt stations, in the period january 2003-may 2004.

V. CONCLUSION

In this paper we have reported on some experiments on NNs based inversions of simulated ESA-Envisat SCIAMACHY UV/VIS radiance data, based upon a sensitivity study performed by means of the LibRadtran suite and of a complementary Extend Pruning process, for tropospheric ozone retrieval purposes. The Nets demonstrated encouraging retrieval capabilities. Starting from this work we tried to use real SCIAMACHY data to train a dedicated NNs algorithm for Tropospheric Ozone Column retrieval. We tested our Net on two midlatitude reference sites. The retrieved TOCs seem to follow the time trend of the reference ozonesondes collocated and simultaneous data, though a systematic underestimation is reported. Even if the results need more investigation, we'd like to stress that the procedure can easily be extended to the spectral measurements of the OMI instrument, carried by the EOS-Aura platform; in this case, the improved horizontal resolution of the sensor could help in monitoring and understanding a number of local and short-range air pollution phenomena.

ACKNOWLEDGMENT

We'd like to acknowledge the owners and providers of WOUDC and SHADOZ ozonesondes data. The authors would like to thank Emanuele Angiuli for figure 5.

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