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The feasibility of retrieving vertical temperature profiles from satellite nadir UV observations: A sensitivity analysis and an inversion experiment with neural network algorithms

P. Sellitto [a,*], F. Del Frate [b]

[a] Laboratoire de Météorologie Dynamique (LMD), UMR8539, Institut Pierre Simon Laplace, UPMC/ENS/CNRS, École Normale Supérieure, 24 Rue Lhomond, F-75231 Paris, France
[b] Earth Observation Laboratory, Tor Vergata University, Via del Politecnico 1, I-00133 Rome, Italy

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ABSTRACT

Atmospheric temperature profiles are inferred from passive satellite instruments, using thermal infrared or microwave observations. Here we investigate on the feasibility of the retrieval of height resolved temperature information in the ultraviolet spectral region. The temperature dependence of the absorption cross sections of ozone in the Huggins band, in particular in the interval 320–325 nm, is exploited. We carried out a sensitivity analysis and demonstrated that a non-negligible information on the temperature profile can be extracted from this small band. Starting from these results, we developed a neural network inversion algorithm, trained and tested with simulated nadir EnviSat-SCIAMACHY ultraviolet observations. The algorithm is able to retrieve the temperature profile with root mean square errors and biases comparable to existing retrieval schemes that use thermal infrared or microwave observations. This demonstrates, for the first time, the feasibility of temperature profiles retrieval from space-borne instruments operating in the ultraviolet.

1. Introduction

The thermodynamic characterization of the atmosphere is necessary for studying and monitoring dynamical, chemical and radiative processes. An important thermodynamic variable is the temperature profile. Remote sensing measurements are important due to the possibility of obtaining spatio-temporally dense data on a regular basis. Remotely sensed height resolved measurements of temperature profile are obtained from both ground-based (e.g., [1,2]) and satellite observations. As for satellites, the thermal infrared (TIR), e.g., [3] and microwave (MW) radiation, e.g., [4], are used to infer the height resolved temperature information.

The temperature dependence of the absorption cross sections of the ozone in the ultraviolet (UV) and visible spectral range has been observed by laboratory measurements, see, e.g., the review of Orphal [5]. Burrows et al. [6] and Chehade et al. [7] analyzed the temperature dependence of the Hartley, Huggins and Chappuis bands cross section, used as reference spectroscopic data for GOME (Global Ozone Monitoring Experiment) and GOME-2 inversion algorithms, respectively. The temperature dependence is particularly strong in the Huggins band (300–370 nm) [6,8], due to changing rotational and vibrational distributions in the electronic ground state [9]. The sensitivity to vertical ozone profiles of the radiance measurements in the Huggins band, due to this temperature dependence, has been exploited in ozone profile inversion schemes using GOME observations [10].

In the present paper we report on a sensitivity analysis and a first inversion exercise to derive the vertical temperature

* Corresponding author. Tel.: +33 6 83 35 09 57.
E-mail address: psellitto@lmd.ens.fr (P. Sellitto).

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profile, at low vertical resolution, from UV/visible satellite radiance observations. The sensitivity of the Earth back-scattered spectra to temperature profiles is analyzed with simulated satellite data, and results are shown and discussed in Section 2. Starting from the outcomes of this sensitivity analysis, we have developed an inversion algorithm based on neural networks (NNs). This algorithm is described in Section 3. The dataset used to develop, train and test the NN algorithm is described in Section 3.2; the selection of the input wavelengths is discussed in Section 3.3; the algorithm configuration is detailed in Section 3.4; results and performances of the retrieval scheme are shown in Section 3.5. Finally, conclusions are given in Section 4.

2. Sensitivity analysis by radiative transfer calculations

As reference data for our sensitivity analysis we use climatological temperature and ozone profiles. Indeed, the concurrent direct sensitivity to ozone must be accounted for, in the UV spectral range. A height resolved climatology of temperature and ozone is described in [11] and available for download at the URL: http://www.iup.uni-bremen.de/gome/o3climatology/. In the following, we will refer to this climatology as the *Lamsal climatology*. The Lamsal climatology is calculated starting from a large set of ozonesondes/radiosondes and satellites measurements. The total ozone is used as a parameter, and profiles are clustered in function of its measured values. In particular, the Lamsal climatology is composed of different seasonal climatological profiles, with their standard deviation, for each 30° latitude interval, sorting the profiles in 30 DU total ozone ranges. For example, the summer–fall mid-latitude set is composed of 7 total ozone intervals (from 220–250 DU to 400–430 DU) and the winter–spring mid-latitude set is composed of 11 total ozone intervals (from 220–250 DU to 520–550 DU). For this study, we restrict our attention to the mid-latitudes. We have used this dynamical/proxy-based climatology to analyze the sensitivity of a simulated satellite UV/VIS radiance measurement to temperature profile variations, as well as to assess the possible screening from ozone profile variations. Indeed, the impact of direct ozone sensitivity on the observed reflectance may mask the variations in reflectance due to the sensitivity to temperature profile variations. For the radiative modelling calculations, we have used the LibRadtran radiative modelling suite [12]. As an independent reference and general baseline, we have used the Air Force Geophysics Laboratory (AFGL) mid-latitude standard temperature and ozone profiles. Among the different possibilities given by the LibRadtran suite, we have chosen the UVSPEC radiative transfer model (RTM) to generate the observed spectra. We have then investigated on the radiances variations when varying the temperature and ozone profiles according to the mentioned 7/11 climatologies (7: summer–fall, 11: winter–spring).

Our study uses the following quantity as a reference:

$$R\left(O_3^{\mathrm{AFGL}}(z), T^{\mathrm{AFGL}}(z), \vec{P}^{\mathrm{AFGL}}\right) = R^{\mathrm{AFGL}} \quad (1)$$

The quantity R^{AFGL} is the radiance spectrum computed with the AFGL temperature and ozone profiles. In Eq. (1), $\vec{P}$ is a vector summarizing the effect of other model parameters as aerosols optical properties and surface albedo. The values of R^{AFGL} have been compared with 2 groups of 7/11 quantities:

$$R\left(O_3^{\mathrm{Lamsal}(n)}(z), T^{\mathrm{AFGL}}(z), \vec{P}^{\mathrm{AFGL}}\right) = R^n_{O_3} \quad (2)$$

$$R\left(O_3^{\mathrm{AFGL}}(z), T^{\mathrm{Lamsal}(n)}(z), \vec{P}^{\mathrm{AFGL}}\right) = R^n_T \quad (3)$$

with $n=1,\ldots,7(11)$ denoting the 7/11 climatologies. The spectra R^{AFGL}, $R^n_{O_3}$ and R^n_T have been computed in the range 220–800 nm by modelling a typical nadir UV/VIS satellite observation geometry, basing on the spectral resolution, the slit function and the operating wavelength of EnviSat SCIAMACHY (SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY) [13]. Then the spectral percent differences have been computed by means of the following quantities:

$$\mathrm{Diff}^n_{O_3} = 100 * \frac{R^n_{O_3} - R^{\mathrm{AFGL}}}{R^{\mathrm{AFGL}}} \quad (4)$$

$$\mathrm{Diff}^n_T = 100 * \frac{R^n_T - R^{\mathrm{AFGL}}}{R^{\mathrm{AFGL}}} \quad (5)$$

Fig. 1 shows the spectral radiance differences of Eqs. (4) and (5), for the 7/11 classes of summer–fall and winter–spring conditions, for both ozone and temperature variations. Here we analyze the summer–fall conditions (Fig. 1c and d). In fact, the interpretation is much clearer on summer–fall conditions, while for winter–spring the spectral differences have more complex dependencies. At shorter wavelengths, the variation caused by the ozone change masks the effect of the temperature variations. At wavelengths higher than 400 nm, the effect of $\vec{P}$ is expected to dominate the interactions with radiation [14]. There is an intermediate region in the Huggins band which is worth more investigation.

We then investigate more closely the 320–325 nm interval, where the ozone cross section is more dependent on the temperature profile [6]. We introduced the following parameter:

$$\mathrm{Diff}^n_{\mathrm{rel}} = \frac{\mathrm{Diff}^n_T}{\mathrm{Diff}^n_{O_3}} = \frac{R^n_T - R^{\mathrm{AFGL}}}{R^n_{O_3} - R^{\mathrm{AFGL}}} \quad (6)$$

$\mathrm{Diff}^n_{\mathrm{rel}}$ is shown in Fig. 2, in the 320–325 nm interval, for the 7/11 total ozone classes. The plots show that, for some of the 7/11 classes, the sensitivity to temperature profile variations is higher than that to ozone profile variations near the wavelengths 321.2 nm and 323.8 nm. This is preferentially observed for the summer–fall dataset, while this property is verified only for the class of 370–400 DU, for the winter–spring dataset.

To better show this behaviour, in Fig. 3 we report the module of the relative sensitivity given by Eq. (6) at 323.8 nm, as a function of total ozone. A similar behaviour is observed at 321.2 nm. Hence, for summer–fall conditions, a reasonable relative sensitivity to temperature exists for moderate values of the total ozone. The sensitivity is scarce for both the highest and lowest values. For winter–spring conditions, this interval of relative sensitivity, and the sensitivity itself, is smaller. It can be remarked that the extreme values are quite uncommon at mid-latitudes [11].