Building Infrastructure for the validation of satellite derived atmospheric parameters: Development of "Phaethon" system

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Executive Summary

Introduction

The project "Building Infrastructure for the validation of satellite derived atmospheric parameters" with the acronym "Phaethon" aimed at developing a low-cost ground based system for the retrieval of column densities of various atmospheric gases, based on a prototype system that was developed for aerosol optical depth and solar radiation measurements (Kouremeti et al., 2008). This system was upgraded by modifying its optical characteristics to fulfill the requirements for atmospheric gas retrievals with the Differential Optical Absorption Spectroscopy (DOAS) technique (Platt and Stutz, 2008).

In DOAS, spectral measurements of solar radiation (radiance) which has been absorbed by atmospheric constituents and then scattered by air molecules are compared with a reference spectrum which has undergone weaker absorption. The differences in the wavelength-dependent absorption features of the two spectra appear as a characteristic differential spectrum of proportional magnitude. This "differential" spectrum is analyzed by least-squares fits of cross sections, after the removal of slowly-varying spectral features by spectral smoothing. Spectrally resolved radiance and irradiance measurements acquired by the Phaethon system are analyzed with the QDOAS algorithm (Fayt and van Roozendael, 2001) to derive differential slant column densities (DSCD) of atmospheric gases. The DSCD is converted to vertical column density with the aid of the airmass factors (AMF) which quantify the enhancement of attenuation of radiation due to absorption and scattering along its atmospheric path. The AMF is derived from radiative transfer model calculations taking into account information on the likely atmospheric composition and structure (e.g., Rozanov and Rozanov, 2010).

The project comprised three major phases:

- 1. The upgrade of the original Phaethon system both in terms of hardware and software
- 2. The validation of the system by comparison to a state of the art MAX-DOAS system
- 3. A pilot application of the system for the validation of corresponding satellite products

Upgrade of Phaethon system

The original Phaethon system was optimized for measurements of spectral solar irradiance and radiance in the spectral region 310-1000 nm, and subsequent retrieval of spectral aerosol optical depth. Details on this system can be found in Kouremeti et al., (2008). The required modifications of the original system were determined by analyzing and comparing its characteristics with those required for achieving higher accuracy in the retrieved quantities. Additionally, the new system was designed to be portable, to take part in validation campaigns, and stable under different meteorological and weather conditions.

The requirements for the upgraded instrument were linked to the corresponding driving scientific factors; hence particular emphasis was given to assessing the effects caused by the spectral range of the measured spectra, the spectral resolution, and the field of view (FOV) of the entrance optics, in relation to the accuracy of the retrieval of columns and, possibly, profiles of certain atmospheric gases. Three of the components of the original Phaethon system were modified: the spectrometer, the entrance optics, and the operating software. To assure stable performance, a temperature control unit was added to the system to stabilize the temperature of the spectrometer and CCD.



Figure 1. Schematic diagram of the layout of the upgraded Phaethon system showing its major components.

The spectrograph of the new system is a Maya 2000 Pro spectrometer manufactured by Ocean Optics, equipped with a back-thinned 2 dimensional FFT-CCD detector (Hamamatsu S10420). It is has high quantum efficiency in the UV where atmospheric radiation intensity is weak. A new 8 m long and 1 mm thick UV graded light-guide, assembled from single quartz glass fibers to a bundle, assures high flexibility and constant light throughput. The new entrance optics result in a 1° field of view which fulfils the requirements for the retrieval of vertical distribution of atmospheric gases. A filter wheel with 8 positions allows the use of different optical components required for the measurements (neutral density and band pass filters, dark signal). A schematic of the system is shown in Figure 1.

The upgraded system was exhaustively tested and evaluated by laboratory and ambient radiation measurements in order to fully characterize its components and the sensitivity and stability of its optical characteristics. A suitable methodology for the rejection of the stray light inside the spectrometer was developed and implemented in the data processing procedures. Moreover, the effect of different aerosol layering in the calculation of air mass factors, which may affect the accuracy in retrieving tropospheric columns, was investigated using aerosol information form a lidar system (Balis et al., 2004).

Validation of Phaethon system

The validation of Phaethon was done at the High Altitude Research Station Jungfraujoch, ~3500 m altitude, where a MAX-DOAS system is operated regularly by the Belgian Institute of Space Aeronomy (BIRA). The campaign lasted for one week in October 2010. The entrance optics of Phaethon and the tracker were mounted on the roof of the observatory, 1 bout 1 m far from BIRA instrument, at a location suitable for performing spectral sky radiance measurements from the zenith down to about -2° elevation angles, as well as, spectral solar irradiance measurements by pointing directly towards the solar disk. With this configuration both instruments were capable in pointing at the same locations on the sky, without obstructing each other (Figure 2).

Zenith sky radiance spectra were acquired at solar zenith angles larger than 85°, both in the morning and in the evening. During the rest of the day, alternating scans of direct solar irradiance and sky radiance at 14 viewing elevation angles and at 315° azimuth angle were recorded by the two systems. Exact synchronization could not be achieved due to differences in the optical characteristics and operational details of the two systems. Lack of exact synchronization introduced occasionally important uncertainties in the comparisons, due to the need for interpolation of data.

For each observation angle, the spectra were analyzed with the QDOAS algorithm in order to retrieve the Differential Slant Column Density (DSCD) of various atmospheric gases, with emphasis in NO₂ and O₄. NO₂ is an important gas particularly in the troposphere over urban or industrial areas, while O₄ is useful in providing information on the aerosols over an area and their influence on the retrieval of NO₂ and other trace gas profiles. Two spectral ranges were used, one in the visible (425-490 nm) and the other in the ultraviolet (338-370 nm). Other gases that absorb mainly in the UV region were also retrieved but with larger errors due to the coarser spectral resolution of the instrument in the UV and due to remaining effects from stray light, which could not be completely removed.

Comparison of the two systems revealed that Phaethon slightly overestimates the derived DSCD of NO₂ systematically, on average by 0.14×10^{16} molec cm⁻², and that its estimates are noisier (Figure 3). This behavior may be attributed to the weak absorption from NO₂ and the



Figure 2. The entrance optics of Phaethon (left) and BIRA MAX-DOAS (center) systems on the roof of the Jung-fraujoch Observatory during the Phaethon validation campaign in October 2010.

resulting uncertainty, which for Phaethon is more significant because its spectrometer is simpler and less accurate compared to BIRA. However, more than 75% of the data agree to within $\pm 0.1 \times 10^{16}$ molec cm⁻², and generally this offset is very small. Despite this positive offset of Phaethon, the two instruments follow closely each other's variations, as the slopes of the regressions are close to unity (within $\pm 5\%$). For twilight, the derived DSCD data represent predominantly absorption by stratospheric NO₂. The morning stratospheric vertical column (VCD) of NO₂ derived from Langley extrapolations is about 2.4 ($\times 10^{16}$ molec cm⁻²) for BIRA and 0.1-0.4 ($\times 10^{16}$ molec cm⁻²) higher for Phaethon. This offset is sustained also for the afternoon columns, which are on average about 1.2 ($\times 10^{16}$ molec cm⁻²) higher for both instruments. To summarize, the average bias between Phaethon and BIRA for the DSCD is about 35-40% ($\pm 20\%$, 1 σ) for the off axis and ~20% ($\pm 10\%$) for the zenith spectra. However, for the slant column density (SCD), the quantity used in most applications, the bias is reduced significantly to 5-10% ($\pm 5\%$) for all viewing angles.

The DSCD of the oxygen dimmer (O₄) was retrieved also from the off-axis and zenith spectral radiances. In contrast to NO₂, the bulk of O₄ is found in the troposphere, where air density is larger. About 60% of O₄ lies below the campaign site. The agreement of Phaethon with BIRA is very good for viewing angles <8°, with deviations ranging from 15-25% at other viewing angles. In general, the comparison of the O₄ DSCD suffers from the weak absorption signal, making difficult to draw firm conclusions on the agreement between the two instruments and on the quality of the O₄ retrievals with Phaethon.



DSCD of NO2 (mol.cm⁻²) retrieved in Visible (425-490 nm)

Figure 3. Scatter plots of NO_2 DSCD measured by Phaethon and BIRA for SZA<85° and for various viewing angles. Different colors refer to different days (DOY 285-blue, 286-cyan, 287-yellow, and 288-red). The intercepts (i) and slopes (s) of the regression lines are shown on each panel. The black solid line is for X=Y.

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Monitoring with Phaethon at Thessaloniki

Direct solar irradiance and sky radiance (zenith and off-axis) spectral measurements are regularly performed at Thessaloniki, Greece, with Phaethon from sunrise to sunset with emphasis in the time period 6:00-12:30 UT which covers the time of satellite overpasses. Atmospheric columns of total ozone, NO₂ and tropospheric NO₂ are derived from the recorded radiation spectra with the QDOAS algorithm.



Figure 4. Scatter plot of total ozone measurements (in DU) from Phaethon and Brewer versus those derived from GOME-2, for the period January-May 2011.

Daily averages of total O₃ derived from Phaethon and a collocated Brewer MKII spectrophotometer correlate very well (r=0.977), suggesting that Phaethon has the potential, with some further improvements to provide accurate total ozone measurements. Comparisons with estimates from the GOME-2 instrument on board MetOp-A satellite, processed with GDP4.4, show that GOME-2 underestimates total ozone by ~2.5% compared to both ground-based instruments (see Figure 4), consistent with the validation results reported in previous studies for Thessaloniki using 3 years of data (Loyola et al., 2011; Balis et al., 2009).

Comparisons of total and tropospheric columns of NO₂ derived from Phaethon and GOME-2 showed that although the agreement is rather poor, there is some correspondence in the day-to-day variability, with a correlation coefficient of daily averages of 0.84, slightly smaller of those reported in earlier studies (Valks et al., 2011). Concerning the tropospheric NO₂ the agreement is worse (r=0.78), with cases where GOME-2 largely underestimates the ground-based measurements, especially when averaging all pixels within 50 km distance from Phaethon's location. These discrepancies are attributed to the large spatial variability of NO₂ due to the localized air pollution sources (e.g., Pinardi et al., 2008).

Similar comparisons of Phaethon with NO_2 estimates from SCHIAMACHY instrument on board Envisat satellite, revealed greater discrepancies, mainly because of the larger subsatellite pixel area, which leads to smoother NO_2 fields for the satellite sensor.

Conclusions

Phaethon was proven to provide satisfactory results in the retrieval of total and tropospheric columns of NO_2 , O_4 and O_3 with acceptable accuracy. However, at this stage it cannot compete with other sophisticated MAX-DOAS systems. At locations with sufficient load of NO_2 ,

as, e.g., over urban and industrial areas Phaethon is expected to have good performance. In this respect its permanent deployment at Thessaloniki would provide useful information on the validation of satellite products. An advantage of Phaethon is its capability to provide atmospheric columns both from direct solar irradiance and sky radiance spectra during the entire day. Consequently it will provide information on the diurnal course of the retrieved columns, information that satellite instruments are unable to deliver at present. In this respect Phaethon may prove a useful supplement to satellite monitoring of tropospheric gases. Extending of Phaethon's capabilities to derive additional products is already possible as the recorded spectra cover already the required spectra ranges. Retrieval of gases absorbing in the UV-B is more difficult, but still possible with reduced accuracy, due to the spectral resolution in this range.

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