Comparison of Ground-Based Tropospheric NO₂ Columns with OMI/Aura Products in the Greater Area of Thessaloniki by Means of an Air Quality Modeling Tool

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Abstract Phaethon is a ground-based MAX-DOAS system, easily deployed at different locations to address specific air quality problems and support satellite validation studies. Three Phaethon systems have been deployed at different sites in the greater area of Thessaloniki, characterized by diverse local pollution levels representing urban, suburban and rural conditions, aiming at linking tropospheric trace-gas modeling with satellite products. Tropospheric NO₂ columns derived at these sites located within an area of about 15 by 30 km, comparable to the size of OMI/Aura pixel, are compared with the satellite retrievals. The OMI/Aura products underestimate the NO_2 in the city centre, representing the average pollution levels in the sub-satellite pixel area which, in the case of Thessaloniki, corresponds mostly to rural conditions. In order to minimize the collocation differences in spatial distribution between satellite and ground-based measurements, the former are adjusted by factors that are calculated by means of a high resolution air quality modeling tool, consisting of WRF meteorological model and CAMx air quality model. This approach shows significant improvement in the comparisons between ground-based and satellite-derived observations.

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1 Introduction

Nitrogen dioxide (NO₂) is a key pollutant in the troposphere, controlling the ozone production and affecting the oxidation capacity and radiative forcing. The main anthropogenic emission source is fossil fuel combustion in vehicle engines and industrial facilities. Consequently, spatial and temporal heterogeneity in NO₂ concentrations is frequently observed in urban and industrial areas. The main NO₂ emission sources in the city of Thessaloniki, Greece are transportation, domestic heating and industrial plants. During the last decades, a stabilization trend is recorded in NO₂ amounts over the city, while the highest NO₂ levels are observed at traffic hotspots in the centre of Thessaloniki (Moussiopoulos et al. 2008).

The monitoring of NO_2 concentrations in the troposphere is widely performed by both ground-based and satellite instruments (Celarier et al. 2008; Hendrick et al. 2014). Satellite sensors provide NO_2 measurements in a larger scale than the ground-based networks and over areas such as oceans and deserts. However, the spatial and temporal resolution of satellite observations is limited by the sensor's footprint and its overpass time, respectively. Several studies suggested that the space-borne observations underestimate the tropospheric NO_2 levels over urban and industrial regions with variable pollution loadings (Celarier et al. 2008).

Three Phaethon MAX-DOAS instruments have been installed at different locations, which are characterized by diverse atmospheric conditions, within the greater area of Thessaloniki and performed tropospheric NO₂ measurements. These observations are compared with OMI/Aura collocations. In order to improve the comparison results, the OMI data are adjusted using factors that are calculated by an air quality modeling system, consisting of CAMx air quality model and WRF meteorological model.

2 Data and Methodology

Phaethon #1 has been operating on the roof of the Physics Department in the Aristotle University of Thessaloniki located at the city centre (urban conditions, UC). Phaethon #2 was installed at a site with rural conditions (RC) near the sea shore about 26 km away from the city from 1 November 2014 to 31 January 2015. Finally Phaethon #3 was installed at the Alexander Technological Educational Institute of Thessaloniki (ATEITH) located in an area with suburban conditions (SC) to the north-west of the city and from 20 January to 11 May 2015.

For the analysis of the scattered light measurements the Differential Optical Absorption Spectroscopy (DOAS) technique was applied using the QDOAS v2.109_3 software developed by BIRA-IASB and S[&]T. The analysis was done in the spectral window 400–450 nm; the broadband absorption features were removed by a 4th degree polynomial; and a second-order linear offset and a Ring effect spectrum, calculated according to Chance and Spurr (1997), were included in

analysis. Along with NO₂, absorption by O₃, O₄ and H₂O were also taken into account. The zenith spectrum of each elevation sequence was used as reference in order to minimize the stratospheric component in the calculated off-axis differential Slant Column Densities (dSCDs) (Hoenninger et al. 2004). The tropospheric vertical column density (VCD) can be calculated for each elevation angle by:

$$VCD_{trop} = \frac{dSCD_{trop}}{dAMF_{trop}}$$
(1)

where the $dAMF_{trop}$ is the tropospheric differential air mass factor which represents the absorption enhancement in the light path.

For the calculation of tropospheric NO₂ AMFs the modelling package libRadtran and a pseudo-spherical discrete ordinate radiative transfer method were used. Typical values were assumed for the aerosol single scattering albedo (0.95), the aerosol asymmetry factor (0.7) and the surface albedo (0.1). Mean vertical profiles were derived by the air quality modelling tool consisting of CAMx and WRF. The mean aerosol optical depth (AOD) vertical profile was derived for the period 2001– 2007 by a LIDAR system operating at LAP (Giannakaki et al. 2010) and was used for all three locations, as suggested by Kazadzis et al. (2009) who found a small spatial variability in AOD and its profile at these locations. The aerosol profile was scaled using different AOD values in the range 0–1.5. AMF look up tables (LUTs) were constructed for each measurement location separately with variables the AOD, the solar zenith angle, and the viewing angles (elevation and azimuth). The AMF corresponding to each measurement is calculated by multi-linear interpolation, using the AOD measurements from the CIMEL sun-photometer operating in LAP/AUTH (http://aeronet.gsfc.nasa.gov/).

The Ozone Monitoring Instrument (OMI) is one of four instruments aboard the NASA EOS-Aura satellite. OMI is a nadir viewing, ultraviolet-visible (270 to 500 nm) imaging spectrometer with pixel size at the nadir 13×25 km that was contributed by the Netherlands and Finland (Levelt et al. 2006). An overpass data set was extracted from OMI/Aura observations for each of the campaign locations. The operational total and tropospheric NO₂ columns are generated by National Aeronautics and Space Administration (NASA) and distributed by the Aura Validation Data Center (AVDC) (http://avdc.gsfc.nasa.gov/).

The air quality modeling tool employed for this study consisted of the Comprehensive Air Quality Model with Extensions (CAMx, version 5.3) (ENVIRON 2010), off-line coupled with the Weather Research and Forecasting—Advanced Research Weather (WRF—ARW, version 3.5.1) (Skamarock et al. 2008). Simulations were carried out for the period November 2014–May 2015 over the grid covering the greater area of Thessaloniki with 2 km spatial resolution. The vertical profile extends up to 10 km above ground-level and contains 22 layers of varying thickness with higher resolution near the ground.

The simulated NO₂ mixing ratio data are available at hourly averaged values per layer for each cell of the domain. These hourly mean vertical profiles of NO₂ concentration were integrated over height and the tropospheric NO₂ VCDs were

estimated. The ratio of the tropospheric NO₂ column of the grid cell that includes the measurement location and the averaged column over the sub-satellite pixel area (7 × 13 cells) OMI measurements in order to minimize the differences between ground-based and satellite observations due to different spatial distribution.

3 Results

The ratios calculated according to the method described above, as well as the reconstructed satellite observations are presented in Fig. 1. In the centre of Thessaloniki (UC) the ratio is in the range 2–2.5 with smaller values observed during winter and higher during spring months. For the other two campaign locations the estimated ratio is much smaller, and it is very close to unit for the RC site. The simulated ratios for the SC location are slightly lower than unit for most



Fig. 1 Hourly ratio of tropospheric NO_2 column to the sub-satellite area averaged column calculated by CAMx for each campaign location (*left panels*). OMI/Aura overpass observations before and after reconstruction using the CAMx ratios (*right panels*)

part of the time series with large variations observed in a few cases. This can be attributed to the fact that this site is located ~ 13 km west of the city centre and due to the pixel footprint size (13×25 km) the OMI measurements can be affected by the heavy loadings observed in the city centre, Hence, the reconstructed OMI overpass data over the SC site are slightly lower than the original.

In Fig. 2 the comparison of ground-based and satellite collocations before and after the OMI data are adjusted is presented. The comparison over the UC area is significantly improved with the slope of the fitted least squares regression line changing from ~ 0.2 to ~ 0.45 . The collocations over the two other campaign locations are generally unaffected by the adjustment, except for a few OMI observations over the SC site that are reduced and this results to a slightly improved comparison with the Phaethon data.



Fig. 2 Time series of tropospheric NO₂ columns from ground-based measurements and satellite overpass data before and after the reconstruction of the latter by means of CAMx simulations (*left*). The same data are shown also as scatter diagrams (*right*)

4 Conclusions

Three Phaethon MAX-DOAS systems have been deployed and performed tropospheric NO₂ column measurements at three locations within the greater area of Thessaloniki, Greece, characterized by different atmospheric pollution loadings. The derived data are compared with OMI/Aura collocations in order to assess the differences in spatial distribution between satellite and ground-based observations. The comparison revealed an average underestimation in tropospheric NO₂ column over the urban area from the satellite sensor of about $6x10^{15}$ molecules/cm² and very good agreement over the other two locations. The OMI data set was reconstructed by means of adjustment factors derived from simulations of an air quality modeling system. The method applied resulted in a significant improvement in collocation comparison over the urban region.

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