File Revision Date:
September 01, 2022

Data Set Description:

PI:	Alkiviadis Bais
Instrument:	Phaethon UV-Visible Spectrometer
Site(s):	LAP.AUTH, Thessaloniki, 40.633° N, 22.956° E
Measurement Quantities:	O3 and NO2

Contact Information:

Name:	Alkiviadis Bais
	Dimitris Karagkiozidis
Address:	Laboratory of Atmospheric Physics
	Aristotle University of Thessaloniki
	54124 Thessaloniki, Greece
Phone:	+30 2310 998 088
Email:	abais@auth.gr/dkaragki@auth.gr

Reference Articles:

Drosoglou, T., Bais, A. F., Zyrichidou, I., Kouremeti, N., Poupkou, A., Liora, N., Giannaros, C., Koukouli, M. E., Balis, D., and Melas, D.: Comparisons of ground-based tropospheric NO2 MAX-DOAS measurements to satellite observations with the aid of an air quality model over the Thessaloniki area, Greece, Atmos. Chem. Phys., 17, 5829–5849, https://doi.org/10.5194/acp-17-5829-2017, 2017.

Drosoglou, T., Koukouli, M. E., Kouremeti, N., Bais, A. F., Zyrichidou, I., Balis, D., van der A, R. J., Xu, J., and Li, A.: MAX-DOAS NO2 observations over Guangzhou, China; ground-based and satellite comparisons, Atmos. Meas. Tech., 11, 2239–2255, https://doi.org/10.5194/amt-11-2239-2018, 2018.

Gkertsi, F., Bais, A., Kouremeti, N., Drosoglou, T., Fountoulakis, I., and Fragkos, K.: DOAS-based total column ozone retrieval from Phaethon system, Atmos. Environ., 180, 51–58, https://doi.org/10.1016/j.atmosenv.2018.02.036, 2018.

Karagkiozidis, D., Friedrich, M. M., Beirle, S., Bais, A., Hendrick, F., Voudouri, K. A., Fountoulakis, I., Karanikolas, A., Tzoumaka, P., Van Roozendael, M., Balis, D., and Wagner, T.: Retrieval of tropospheric aerosol, NO2, and HCHO vertical profiles from MAX-DOAS observations over Thessaloniki, Greece: intercomparison and validation of two inversion algorithms, Atmos. Meas. Tech., 15, 1269–1301, https://doi.org/10.5194/amt-15-1269-2022, 2022.

Koukouli, M.-E.; Pseftogkas, A.; Karagkiozidis, D.; Skoulidou, I.; Drosoglou, T.; Balis, D.; Bais, A.; Melas, D.; Hatzianastassiou, N. Air Quality in Two Northern Greek Cities Revealed by Their Tropospheric NO2 Levels. Atmosphere 2022, 13, 840. https://doi.org/10.3390/atmos13050840.

Kouremeti, N., Bais, A., Kazadzis, S., Blumthaler, M., and Schmitt, R.: Charge-coupled device spectrograph for direct solar irradiance and sky radiance measurements, Appl. Optics, 47, 1594–607, 2008.

Kouremeti, N., Bais, A. F., Balis, D., and Zyrichidou, I.: Phaethon, A System for the Validation of Satellite Derived Atmospheric Columns of Trace Gases, in: Advances in Meteorology, Climatology and Atmospheric Physics, edited by: Helmis, C. G. and Nastos, P. T., Springer, Berlin, Heidelberg, 1081–1088, https://doi.org/10.1007/978-3-642-29172-2_151, 2013.

Kreher, K., Van Roozendael, M., Hendrick, F., Apituley, A., Dimitropoulou, E., Frieß, U., Richter, A., Wagner, T., Lampel, J., Abuhassan, N., Ang, L., Anguas, M., Bais, A., Benavent, N., Bösch, T., Bognar, K., Borovski, A., Bruchkouski, I., Cede, A., Chan, K. L., Donner, S., Drosoglou, T., Fayt, C., Finkenzeller, H., Garcia-Nieto, D., Gielen, C., Gómez-Martín, L., Hao, N., Henzing, B., Herman, J. R., Hermans, C., Hoque, S., Irie, H., Jin, J., Johnston, P., Khayyam Butt, J., Khokhar, F., Koenig, T. K., Kuhn, J., Kumar, V., Liu, C., Ma, J., Merlaud, A., Mishra, A. K., Müller, M., Navarro-Comas, M., Ostendorf, M., Pazmino, A., Peters, E., Pinardi, G., Pinharanda, M., Piters, A., Platt, U., Postylyakov, O., Prados-Roman, C., Puentedura, O., Querel, R., Saiz-Lopez, A., Schönhardt, A., Schreier, S. F., Seyler, A., Sinha, V., Spinei, E., Strong, K., Tack, F., Tian, X., Tiefengraber, M., Tirpitz, J.-L., van Gent, J., Volkamer, R., Vrekoussis, M., Wang, S., Wang, Z., Wenig, M., Wittrock, F., Xie, P. H., Xu, J., Yela, M., Zhang, C., and Zhao, X.: Intercomparison of NO2, O4, O3 and HCHO slant column measurements by MAX-DOAS and zenith-sky UV–visible spectrometers during CINDI-2, Atmos. Meas. Tech., 13, 2169–2208, https://doi.org/10.5194/amt-13-2169-2020, 2020.

Liu, S., Valks, P., Pinardi, G., Xu, J., Chan, K. L., Argyrouli, A., Lutz, R., Beirle, S., Khorsandi, E., Baier, F., Huijnen, V., Bais, A., Donner, S., Dörner, S., Gratsea, M., Hendrick, F., Karagkiozidis, D., Lange, K., Piters, A. J. M., Remmers, J., Richter, A., Van Roozendael, M., Wagner, T., Wenig, M., and Loyola, D. G.: An improved TROPOMI tropospheric NO2 research product over Europe, Atmos. Meas. Tech., 14, 7297–7327, https://doi.org/10.5194/amt-14-7297-2021, 2021.

Pinardi, G., Van Roozendael, M., Hendrick, F., Theys, N., Abuhassan, N., Bais, A., Boersma, F., Cede, A., Chong, J., Donner, S., Drosoglou, T., Dzhola, A., Eskes, H., Frieß, U., Granville, J., Herman, J. R., Holla, R., Hovila, J., Irie, H., Kanaya, Y., Karagkiozidis, D., Kouremeti, N., Lambert, J.-C., Ma, J., Peters, E., Piters, A., Postylyakov, O., Richter, A., Remmers, J., Takashima, H., Tiefengraber, M., Valks, P., Vlemmix, T., Wagner, T., and Wittrock, F.: Validation of tropospheric NO2 column measurements of GOME-2A and OMI using MAX-DOAS and direct sun network observations, Atmos. Meas. Tech., 13, 6141–6174, https://doi.org/10.5194/amt-13-6141-2020, 2020.

Tirpitz, J.-L., Frieß, U., Hendrick, F., Alberti, C., Allaart, M., Apituley, A., Bais, A., Beirle, S., Berkhout, S., Bognar, K., Bösch, T., Bruchkouski, I., Cede, A., Chan, K. L., den Hoed, M., Donner, S., Drosoglou, T., Fayt, C., Friedrich, M. M., Frumau, A., Gast, L., Gielen, C., Gomez-Martín, L., Hao, N., Hensen, A., Henzing, B., Hermans, C., Jin, J., Kreher, K., Kuhn, J., Lampel, J., Li, A., Liu, C., Liu, H., Ma, J., Merlaud, A., Peters, E., Pinardi, G., Piters, A., Platt, U., Puentedura, O., Richter, A., Schmitt, S., Spinei, E., Stein Zweers, D., Strong, K., Swart, D., Tack, F., Tiefengraber, M., van der Hoff, R., van Roozendael, M., Vlemmix, T., Vonk, J., Wagner, T., Wang, Y., Wang, Z., Wenig, M., Wiegner, M., Wittrock, F., Xie, P., Xing, C., Xu, J., Yela, M., Zhang, C., and Zhao, X.: Intercomparison of MAX-DOAS vertical profile retrieval algorithms: studies on field data from the CINDI-2 campaign, Atmos. Meas. Tech., 14, 1–35, https://doi.org/10.5194/amt-14-1-2021, 2021.

Roscoe, H.K., et al., Intercomparison of slant column measurements of NO2 and O4 by MAX-D0AS and zenith-sky UV and visible spectrometers, Atmos. Meas. Tech., 3, 1629-1646, 2010.

Vandaele, A.C., et al., An intercomparison campaign of ground-based UV-Visible measurements of NO2, BrO, and OClO slant columns. I. Methods of analysis and results for NO2, J. Geophys. Res., 110, D08305, doi:10.1029/2004JD005423, 2005.

Van Roozendael, M., et al., Validation of Ground-Based Visible Measurements of Total Ozone by Comparison with Dobson and Brewer Spectrophotometers, J. Atm. Chem., 29, 55-83, 1998.

Verhoelst, T., Compernolle, S., Pinardi, G., Lambert, J.-C., Eskes, H. J., Eichmann, K.-U., Fjæraa, A. M., Granville, J., Niemeijer, S., Cede, A., Tiefengraber, M., Hendrick, F., Pazmiño, A., Bais, A., Bazureau, A., Boersma, K. F., Bognar, K., Dehn, A., Donner, S., Elokhov, A., Gebetsberger, M., Goutail, F., Grutter de la Mora, M., Gruzdev, A., Gratsea, M., Hansen, G. H., Irie, H., Jepsen, N., Kanaya, Y., Karagkiozidis, D., Kivi, R., Kreher, K., Levelt, P. F., Liu, C., Müller, M., Navarro Comas, M., Piters, A. J. M., Pommereau, J.-P., Portafaix, T., Prados-Roman, C., Puentedura, O., Querel, R., Remmers, J., Richter, A., Rimmer, J., Rivera Cárdenas, C., Saavedra de Miguel, L., Sinyakov, V. P., Stremme, W., Strong, K., Van Roozendael, M., Veefkind, J. P., Wagner, T., Wittrock, F., Yela González, M., and Zehner, C.: Ground-based validation of the Copernicus Sentinel-5P TROPOMI NO2 measurements with the NDACC ZSL-DOAS, MAX-DOAS and Pandonia global networks, Atmos. Meas. Tech., 14, 481–510, https://doi.org/10.5194/amt-14-481-2021, 2021.

<u>Instrument Description:</u>
Since 2018, two UV/Vis zenith-sky spectrometers (type Phaethon) have been operating at the Laboratory of Atmospheric Physics, Thessaloniki, Greece for the retrieval of NO2 and O3 columns. Their technical characteristics and specifications are described below.

Instrument identification number: Phaethon 7 (2018 - 2022):
Spectrometer: AvaSpec-ULS2048LTEC (f=75 mm)
Entrance slit: 50 microns
Grating: 1800 grooves/mm
Wavelength range: 297 – 458 nm
Spectral resolution: 0.45 nm FWHM
Detector: Sony ILX511
Temperature: 5° C
Input optic: 8 m Quartz fiber
Field of view: 1°
Instrument automatic control: Custom-made

Instrument identification number: Phaethon 8 (2020 - present):
Spectrometer: AvaSpec-ULS2048x64-EVO (f=75 mm)

Entrance slit: 50 microns
Grating: 1200 grooves/mm
Wavelength range: 275 – 539 nm
Spectral resolution: 0.55 nm FWHM
Detector: Hamamatsu Hams11071-2048x64
Temperature: 10° C
Input optic: 8 m Quartz fiber
Field of view: 1°
Instrument automatic control: Custom-made

Phaethon in a mini custom-built system, developed at the Laboratory of Atmospheric Physics (LAP) that consists of an outdoor telescope, mounted on a two-axis sun-tracker, and an indoor unit (spectrometer). Both systems, operating at LAP, perform spectral measurements from sunrise to sunset up to a solar zenith angle (SZA) of 95°, with acquisition integration times that range between 1 and 3 min depending on the light intensity conditions. They operate in three different measurement modes: Zenith-sky, Off-axis, and Direct-sun. In order to achieve higher signal-to-noise and to avoid saturated spectra, the number of scans of each individual measurement and the exposure time of the CCD are automatically adjusted by the operating software according to the light intensity received by the detector. Dark spectra are measured on a daily basis (after each sequence of scans) and they are subtracted from the radiation spectra. The measured raw data are transferred to a local server in near-real-time through the Internet for spectral analysis and storage.

Algorithm Description:
Both NO2 and O3 slant column densities are retrieved by the differential optical absorption spectroscopy (DOAS) analysis of the measured radiance spectra using the QDOAS software that is developed by IASB-BIRA. NO2 is analyzed in the 411-445 nm and 425-490 nm spectral windows for Phaethon 7 and Phaethon 8, respectively. O3 is retrieved only for the Phaethon 8 system in the window 450 - 540 nm (in the Chappuis band). The vertical columns are derived from measured slant columns using look-up tables of air mass factors (AMFs), following the new NDACC recommendations available at http://uv-vis.aeronomie.be/groundbased/. For NO2, these are based on a harmonic climatology of stratospheric NO2 profiles, while for ozone the TOMS V8 O3 profile climatology is being used. Mean twilight vertical columns are obtained by averaging individual measurements between 86 and 91° SZA.

Expected Precision/Accuracy of Instrument:
The error budget of the measurements is obtained by considering error sources affecting the determination of the slant column densities (SCD), the residual amount in the reference spectrum (R), and the air mass factor (AMF). Fitting errors derived from the least-squares analysis typically give small uncertainties of the order of 3E14 molec/cm2 for NO2 SCDs and 5 DU for O3 SCDs. However, results from intercomparisons exercises (e.g., Van Roozendael et al., 1998; Vandaele et al., 2005; Roscoe et al., 2010) show that state-of-the-art instruments hardly agree to better than a few percent, even using standardized analysis procedures, which indicates that the actual accuracy on SCDs is limited by uncontrolled instrumental and/or analysis factors. More conservatively, and including uncertainties of absorption cross-sections and their temperature dependencies, we quote an uncertainty of the order 5% for NO2 SCDs, and 2% for O3 SCDs. The accuracy on R is mostly limited by the method used to derive

the vertical column at the time of the reference spectrum acquisition (we use a Langley-plot approach). The contribution from this error source to the total error budget is generally small (typically 1-2%), although it may become significantly larger for NO_2 when very low abundances are to be monitored. In most conditions, the major contribution to the error budget of both NO_2 and O_3 total columns is the AMF calculation which requires appropriate modelling of the diffuse radiance in the nadir direction. Published studies indicate that the sensitivity of the AMF to stratospheric profiles of pressure, temperature and the constituent itself accounts for an uncertainty of 10 % maximum for NO_2, and 4 % for O_3. In the case of NO_2, much larger errors can be obtained when tropospheric NO_2 is produced or transported above the station. Such pollution events are usually easily detected by inspection of the SZA dependency of the NO_2 SCDs and are filtered out in the analysis process. In summary we estimate the total accuracy on vertical columns to be in most cases better than 15% for NO_2, and better than 5% for O_3.

Instrument History:
starting date: 2018/01/01
ending date: 2022/06/22
spectrometer 1:
AvaSpec-ULS2048LTEC, grating 1800 grooves/mm, 297-458 nm, FWHM 0.45 nm
Entrance slit 50 microns, Sony ILX511 detector (5° C)

---

starting date: 2020/05/28
ending date: present
spectrometer 1:
AvaSpec-ULS2048x64-EVO, grating 1200 grooves/mm, 275-539 nm, FWHM 0.55 nm
Entrance slit 50 microns, Hamamatsu Hams11071-2048x64 detector (10° C)

The Phaethon 7 system has been tested and validated during the Cabauw Intercomparison of Nitrogen Dioxide Measuring Instruments 2 (CINDI-2) campaign in 2016 in Cabauw, the Netherlands.
The Phaethon 8 system has been tested and validated against measurements of Phaethon 7.