File Revision Date:
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Data Set Description:

PI:	Michel Van Roozendael
Instrument:	SAOZ and MAX-DOAS UV-Vis spectrometers
Site(s):	Jungfraujoch, 46°N, 8°E
Measurement Quantities:	Total Ozone, total stratospheric NO2
Data revision:	2023

Contact Information:

Name:	Michel VAN ROOZENDAEL/Alexis Merlaud/Caroline Fayt/ Francois Hendrick
Address:	3 avenue Circulaire, B-1180 Brussels, Belgium
Phone:	+32 2 3730416
Email:	michel.vanroozendael@aeronomie.be/caroline.fayt@aeronomie.be/ alexis.merlaud@aeronomie.be/francois.hendrick@aeronomie.be

Reference Articles:

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.

Franco, B., Hendrick, F., Van Roozendael, M., Müller, J.-F., Stavrakou, T., Marais, E. A., Bovy, B., Bader, W., Fayt, C., Hermans, C., Lejeune, B., Pinardi, G., Servais, C., and Mahieu, E.: Retrievals of formaldehyde from ground-based FTIR and MAX-DOAS observations at the Jungfraujoch station and comparisons with GEOS-Chem and IMAGES model simulations, Atmos. Meas. Tech., 8, 1733-1756, doi:10.5194/amt-8 1733-2015, 2015.

Hendrick, F., E. Mahieu, G. Bodeker, K. F. Boersma, M. P. Chipperfield, M. De Mazière, P. Demoulin, I. De Smedt, C. Fayt, C. Hermans, K. Kreher, B. Lejeune, G. Pinardi, C. Servais, J.-P. Vernier, and M. Van Roozendael, Trend analysis of stratospheric NO2 at Jungfraujoch (46.5°N, 8.0°E) using ground-based UV-visible, FTIR, and satellite nadir observations, Atmos. Chem. Phys., 12, 8851–8864, 2012.

Hendrick, F., J.-P. Pommereau, F. Goutail, R. D. Evans, D. Ionov, A. Pazmino, E. Kyrö, G. Held, P. Eriksen, V. Dorokhov, M. Gil, and M. Van Roozendael, NDACC/SAOZ UV-visible total ozone measurements: Improved retrieval and comparison with correlative ground-based and satellite observations, Atmos. Chem. and Phys., 11, 5975-5995, 2011

Instrument Description:

Three UV/Vis measurements systems have been successively operated at the Jungfraujoch:

1) 1991-2014: a SAOZ zenith-sky spectrometer for NO2 and O3 total columns,
2) 2010-2019/2023-now: a MAX-DOAS instrument providing complementary total columns of ozone and NO2, stratospheric BrO as well as tropospheric measurements of HCHO, NO2
3) 2022-now: a miniSAOZ system developed at BIRA as a successor of the SAOZ instrument.

SAOZ:

The SAOZ (Systeme d'Analyse par Observations Zenithales) is made of a commercial Jobin-Yvon CP200 flat field spectrometer equipped with a holographic grating and an Hamamatsu diode array detector. The resolution is of the order of 1 nm in the range 300-600 nm. Three versions have been used at the Jungfraujoch (see below). In the first version, a 200 gr/mm grating was associated to a 512 diode array detector and a 25 micron entrance slit. In the second version, a 360 gr/mm grating was associated to a 1024 diode array detector and a 50 micron entrance slit. The third version was equipped with a 1024 diode array detector also from Hamamatsu, featuring lower noise and allowing for better sampling of the NO2 and O3 differential absorption spectrum. The equipment is operated outside, placed in a dust-and-water proof container. Zenith-sky light is collected within a total field of view of 10°. Measurements are performed from sunrise to sunset up to a Solar Zenith Angle (SZA) of 94°. The data are transmitted to BIRA-IASB in near-real-time through the Internet.

MAX-DOAS:

The BIRA-IASB MAX-DOAS is a custom-build dual-channel system consisting of an outdoor optical head mounted on a sun-tracker, and an indoor spectrometric unit. Two optical fibers with rectangular terminations link the optical head with the two spectrometers. The optical head design is mounted on a commercial sun tracker from the BRUSAG company (INTRA), which is used to collect direct solar irradiance or scattered skylight by means of an off-axis parabolic mirror within a 0.8 deg field of view.

The first spectrometer from ORIEL (MS260i 1/4m), covers the UV region (298-387 nm) with a grating of 1200 grooves/mm blazed at 350 nm, leading to a spectral resolution of 0.4 nm FWHM. A bandpass filter (U340 HOYA) is used to block the visible light at the entrance slit of the spectrometer hence reducing stray-light at UV wavelengths. This spectrometer is equipped with a thermoelectrically-cooled (-50 deg C) back illuminated UV-enhanced CCD detector from Princeton Instruments (model PIXIS 2KBUV) featuring 2048x512 pixels. The second channel uses an ORIEL MS127 spectrometer covering the spectral range from 406 to 556 nm at a resolution of 0.6 nm FWHM. It is also equipped with a CCD detector from Princeton Instruments (model Spec-10:100B) cooled to -50 deg C. The whole system is mounted inside a thermally regulated container to minimize thermal stress on mechanical and optical parts. The data acquisition is controlled by computer and the spectral measurements are transferred daily to BIRA for quality control and data processing.

miniSAOZ:

The miniSAOZ instrument is made of an optical head, fixed to the guardrail on the terrace of the observatory and of a commercial grating spectrometer unit installed inside the laboratory and connected to the head using an optical fiber. The field of view at zenith is constrained to about 6° full angle by means of a lens. The spectrometer is an Avantes AvaSpec-HERO built around a High-Sensitivity 100mm optical bench offering a NA of 0.13 featuring a cooled (-10°C), back-thinned detector of 1024×58 pixels. A spectral range from 385 to 560 nm is covered with a resolution of 0.4nm FWHM between 430 and 500 nm. The data acquisition is controlled using a home-made software, allowing for fully automatic measurements during the whole day until reaching 92° of solar zenith angle. Spectral data are transferred daily to BIRA for further processing.

<u>Algorithm Description:</u>

The spectral evaluation of both SAOZ and MAX-DOAS (zenith-sky) data is performed using the QDOAS software. NO2 is analysed in the 425-490 nm spectral window, and ozone from 450 to 550 nm. Vertical columns are derived from measured slant columns using look-up tables of air mass factors (AMFs), following the NDACC recommendations available on http://uv-vis.aeronomie.be/ groundbased/. For NO2, these are based on an harmonic climatology of stratospheric NO2 profile, 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.

<u>Expected Precision/Accuracy of Instrument:</u>

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 NO2 when very low abundances are to be monitored. In most conditions, the major contribution to the error budget of both NO2 and O3 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:

SAOZ-512 (PCD detector): start Jun 1990 - end May 1991
SAOZ-512 (NMOS detector): start Nov 1991 - end May 1998

SAOZ-1024:

- start Nov 1998 - end Apr 1999
- start Jul 1999 - end Dec 1999
- start Feb 2000 - end Apr 2000
- start Nov 2001 - end Feb 2006
- start Apr 2006 - end May 2006
- start Sep 2006 - end May 2007
- start Aug 2008 - end May 2009
- start Sep 2009 - end Apr 2010
- start Jun 2010 - end Aug 2010
- start Dec 2010 - end Jun 2014

MAX-DOAS (Visible channel):

- start Jul 2010 - end Nov 2013
- start Mar 2014 - end Jun 2016

MAX-DOAS (UV channel):

- start Jul 2010 - end Nov 2013
- start Mar 2014 - end Feb 2017
- start Jul 2017 - end Jun 2019
- start Aug 2023 - now

miniSAOZ:

- start Apr 2022 - now