File Revision Date:
July 7, 2026

Data Set Description:

PI:	Michel Van Roozendael
Instrument:	SAOZ and MAX-DOAS UV-Vis spectrometers
Site(s):	Jungfraujoch, 46°N, 8°E, 3463 m a.s.l.
Measurement Quantities:	Total Ozone, stratospheric NO_2, tropospheric NO_2 and tropospheric HCHO
Data revision:	2026
Licence type:	CC-BY-4.0
DOIs:	
NO_2 – bira.iasb014	10.60897/ndacc.jungfraujoch_uvvis.doas.zenith.no2_bira.iasb014

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Reference Articles:

Van Roozendael, M., Hendrick, F., Friedrich, M. M., Fayt, C., Bais, A., Beirle, S., Bösch, T., Comas, M. N., Friess, U., Karagkiozidis, D., Kreher, K., Merlaud, A., Pinardi, G., Piters, A., Prados-Roman, C., Puentedura, O., Reischmann, L., Richter, A., Tirpitz, J.-L., Wagner, T., Yela, M., Ziegler, S.; Fiducial Reference Measurements for Air Quality Monitoring Using Ground-Based MAX-DOAS Instruments (FRM4DOAS). Remote Sensing, Vol. 16, Page 4523, 16(23), 4523. https://doi.org/10.3390/RS16234523, 2024.

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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.

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

1) 1991-2014: a SAOZ zenith-sky spectrometer for NO_2 and O_3 total columns,
2) 2010-2019/2023-now: a MAX-DOAS instrument providing complementary total columns of ozone and NO_2, stratospheric BrO as well as tropospheric measurements of HCHO, NO_2
3) 2022-now: a mini-SAOZ system developed at BIRA as a successor of the SAOZ instrument.

SAOZ:
The SAOZ (Zenithal Observation Analysis System) consists of a Jobin-Yvon CP200 commercial flat-field spectrometer fitted with a holographic grating and a Hamamatsu diode array detector. The resolution is of the order of 1 nm in the 300–600 nm range. Three versions were used at the Jungfraujoch. In the first version (1990–1991), a 200 gr/mm diffraction grating was combined with a 512-diode array detector and a 25-micron entrance slit. In the second version (1992–1998), a 360 gr/mm diffraction grating was combined with a 1024-diode barrette detector and a 50-micron entrance slit. The third version (1998–2014) was fitted with a 1024-diode array detector, also manufactured by Hamamatsu, which had lower noise levels. The equipment operated outdoors, housed in a dust- and water-tight container. Zenithal light was collected within a total field of view of 10°.

MAX-DOAS:
The BIRA-IASB MAX-DOAS instrument is a research-grade dual-channel system comprising an outdoor optical head mounted on a solar tracker and an indoor spectrometric unit. Two optical fibres with rectangular ends connect the optical head to the two spectrometers. The optical head is mounted on a commercial sun tracker from BRUSAG. It captures the direct solar radiation or the diffuse sky light within a field of view of 0.8 degrees.

The first spectrometer, supplied by ORIEL (MS260i 1/4 m), covers the UV region (298–387 nm). It is mounted with a diffraction grating of 1200 lines/mm blazed at 350 nm, which provides a spectral resolution of 0.4 nm (FWHM). A bandpass filter (U340 HOYA) is used to block visible light at the spectrometer's entrance slit, thereby reducing stray light in the UV wavelengths. This spectrometer is fitted with a thermoelectrically cooled (-50 °C) back-illuminated CCD detector optimised for UV, manufactured by Princeton Instruments (model PIXIS 2KBUV).

The second channel uses an ORIEL MS127 spectrometer covering the spectral range from 406 to 556 nm with a resolution of 0.6 nm. It is also fitted with a CCD detector from Princeton Instruments (model Spec-10:100B) cooled to -50 °C.

The entire system is housed within a thermally controlled enclosure to minimise thermal stress on the mechanical and optical components. Data acquisition is computer-controlled and the spectral measurements are transferred daily to the BIRA for quality control and data processing.

Mini-SAOZ:

The mini-SAOZ instrument consists of an optical head fixed to the guardrail on the terrace of the observatory and of a commercial grating spectrometer unit. The latter is installed in the Sphynx building 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 by software and allows for automatic measurements during the day until 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. NO_2 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 NO_2, these are based on a harmonic climatology of stratospheric NO2 profile, while for ozone the TOMS V8 O_3 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 random uncertainties of the order of 3e14 molec/cm^2 for NO_2 SCDs and 5 DU for O_3 SCDs. Accounting for uncertainties in absorption cross-sections and their temperature dependencies, we quote an uncertainty of the order 5% for NO_2 SCDs, and 2% for O_3 SCDs. The accuracy on R is typically small (1-2%) but it becomes larger for NO_2 when 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. Pollution events that may degrade the accuracy of the stratospheric NO_2 retrieval 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.

<u>Instrument History:</u>

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
(interruption during 4 years)
start Aug 2023 - now

mini-SAOZ:
start Apr 2022 - now