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September 12, 2025

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 NO₂, tropospheric NO₂ and tropospheric HCHO
Data revision: 2025

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DOIs:

NO₂ – bira.iasb014 10.60897/ndacc.jungfraujoch_uvvis.doas.zenith.no2_bira.iasb014

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Reference Articles:

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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 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 mini-SAOZ system developed at BIRA as a successor of the SAOZ instrument.

SAOZ:

The SAOZ (Système d'Analyse par Observations Zenithales) is made of a commercial Jobin-Yvon CP200 flat field spectrometer equipped with a holographic grating and a Hamamatsu diode array detector. The resolution is of order 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-built 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.

Mini-SAOZ:

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 1024x58 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.

Algorithm Description:

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 a 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.

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 Roozendaal 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. Accounting for uncertainties in 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 NO₂, and 4 % for O₃. Pollution events that may degrade the accuracy of the stratospheric NO₂ retrieval are usually easily detected by inspection of the SZA dependency of the NO₂ 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 NO₂, and better than 5% for O₃.

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

mini-SAOZ:

start Apr 2022 - now