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Data Set Description:

PI: Udo Frieß, Heidelberg University, Germany
CO-PIs: Richard Querel and Dan Smale, NIWA, New Zealand
Instrument: UV-Vis MAX-DOAS
Site(s): Arrival Heights, Antarctica, 77.83°S, 166.67°E, E 184m
Measurement Quantities: Ozone, NO₂
Data Version description:

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Reference Articles:

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- U. Frieß et al., “MAX-DOAS O₄ measurements: A new technique to derive information on atmospheric aerosols: 2. Modeling studies,” *J. Geophys. Res.*, vol. 111, no. 14203, Art. no. 14203, 2006, doi: 10.1029/2005JD006618.
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- Roozendaal, M. V. and Hendrick, F.: Recommendations for total ozone retrieval from NDACC zenith-sky UV-VIS spectrometers, Belgian Institute for Space Aeronomy (BIRA-IASB). [online] Available from: https://uv-vis.aeronomie.be/groundbased/NDACC_UVVIS-WG_O3settings_v2.pdf, 2009.
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J.-L. Tirpitz et al., “Intercomparison of MAX-DOAS vertical profile retrieval algorithms: studies on field data from the CINDI-2 campaign,” *Atmospheric Measurement Techniques*, vol. 14, no. 1, Art. no. 1, 2021, doi: 10.5194/amt-14-1-2021.

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Instrument Description:

The instrument consists of two separate spectrograph/detector units for the UV and Vis wavelength range, located in a single stainless steel housing. The optical parts of the spectrograph are mounted in a ‘sandwich’ design between 3 and 5mm thick stainless steel plates which ensure a high mechanical stability. The housing is evacuated ($p < 10^{-5}$ mBar) and filled with dry argon under slight over-pressure to avoid any freezing or condensation of water onto the cooled detector surfaces. At the fiber bundles exit, the 14 quartz fibers are arranged as columns, serving as entrance slits. The light is dispersed in each spectrograph using concave holographic gratings and is detected with photo diode arrays. The characteristics of both spectrometer units are as follows:

	UV	Vis
Grating Manufacturer	Yobin Yvon	American Holographics
Grating Diameter [mm]	70	85
Focal length [mm]	210	160
Aperture ratio	f/3.2	f/2
Grooves/mm	1200	510
Diffraction order	-1	1
Wavelength range [nm]	320 - 420	400 – 650
Average resolution (FWHM) [nm/channel]	0.5/5.0	1.8/7.2

To avoid any changes in the optical adjustments and to improve the detector cooling, the housing is located inside a custom build fridge that keeps the system on a stable temperature of +2°C. The light dispersed by the holographic gratings is detected using photo diode arrays (PDAs) manufactured by Hamamatsu (type ST3904-1024). The detectors are thermoelectrically cooled to a temperature of -35°C. The dark current signal and electronic offset amount to ≈ 0.25 counts/sec and ≈ 700 counts/scan, respectively.

The telescope consists of a motorised aluminium-coated mirror system (solar tracker) mounted on the roof of the building which reflects the scattered sunlight onto two indoor telescope units for both spectrographs. Here the light is focussed onto the entrances of quartz fibre bundles that conduct the light into the spectrograph units. The telescope is equipped with a lamp housing for regular

measurements of calibration spectra. Since October 2012, scattered skylight is measured a fixed azimuth angle of 304.5° and at elevation angles of 90°, 20°, 10°, 5°, 2°, 1°, 0°, and -4° (the latter angle pointing downwards observing light scattered by the sea ice surface, enhancing the sensitivity for the atmosphere below the instrument's altitude). Before October 2012, measurements were always taken at a fixed relative azimuth angle (RAA) between line of sight and the Sun of 20°, but with varying elevation angle sequences (see Instrument History below).

Algorithm Description:

Spectra are analysed using the DOASIS software developed at the Institute of Environmental Physics of the University of Heidelberg using a non-linear least squares fitting routine based on the Levenberg-Marquardt algorithm.

Ozone slant column densities are retrieved in the wavelength range between 450 and 550 nm according to the recommendations for total ozone retrieval from NDACC zenith-sky UV-VIS spectrometers (v2) [Rozendael and Hendrick, 2009]. Slant column densities are converted to vertical column densities according to the NDACC recommendations using the NDACC AMF data base, with the reference SCD being determined using the Langley plot method.

The spectral retrieval of NO₂ dSCDs is performed in the wavelength region between 425 and 490 nm according to the recommendations for NO₂ column retrieval from NDACC zenith-sky UV-VIS spectrometers (v3) [Rozendael and Hendrick, 2012], and converted to VCDs using the NDACC AMF lookup table.

Expected Precision/Accuracy of Instrument:

Average random errors resulting from spectral noise amount to 4.5 DU for the ozone VCD and 3×10^{13} molec/cm² for the NO₂ VCD. In addition, the accuracy is affected by several systematic error sources. Inaccuracies in the spectral fit, caused by inaccurate cross sections, non-perfect removal of the effects caused by inelastic scattering (Ring effect), wavelength calibration and instrumental artefacts, is expected to lead to an additional uncertainty in the order of 2% for ozone and 5% for NO₂. Although considered in the NDACC AMF lookup tables, uncertainties in the vertical distribution of the trace gases lead to an uncertainty in the airmass factors, which can be estimated to contribute to the VCD error in the order of 4% for ozone and at most 10% for NO₂. Uncertainties in stratospheric photochemistry leads to additional uncertainties of the NO₂ AMF. Furthermore, the uncertainty in the residual trace gas amount of the reference spectrum determined by the Langley plot adds to the error budget with a small contribution of 1-2%. The measurements at Arrival Heights in the pristine Antarctic atmosphere is mostly unaffected by tropospheric pollution, but the influence of emissions from the nearby McMurdo station cannot be completely excluded.

Instrument History:

08/1998: Installation of the DOAS instrument at Arrival Heights, Antarctica.

History of elevation angle sequences:

Start date	Stop date	Azimuth	Elevation sequence			
1998	23.01.2001	20° RAA	10			
23.01.2001	21.03.2001	20° RAA	90	45	20	10
21.03.2001	26.10.2002	20° RAA	90	20	15	10
26.10.2002	22.10.2004	20° RAA	90	20	15	10 2

22.10.2004	23.10.2012	20° RAA	90	20	15	10	5	2		
23.10.2012	present	304.5° Fix	90	20	10	5	2	1	0	-4