

File Revision Date:

April 6, 2021

Data Set Description:

PI: Geraint VAUGHAN
Instrument: SAOZ
Site: Aberystwyth (52.417°N, 4.066°W, 90m.a.s.l)
Measurement Quantities: Total Ozone am, Total Ozone pm, NO₂am, NO₂pm

Contact Information:

Name: John Rimmer/ Andrew Smedley
Address: University of Manchester
Phone: +44 161 306 3906
FAX: +44 161 306 3951
Email: john.rimmer@manchester.ac.uk/ andrew.smedley@manchester.ac.uk

Reference Articles:

Pommereau, J.P. and F. Goutail. Stratospheric O₃ and NO₂ Observations at the Southern Polar Circle in Summer and Fall 1988. Geophys. Res. Lett. 895, 1988.

A. C. Green, L. M. Bartlett and G. Vaughan. SAOZ measurements of total ozone at Aberystwyth. J. Quant. Spec. Radiat. Transfer 69, 231-243, 2001.

G. Vaughan, P. T. Quinn, A. C. Green, J. Bean, H. K. Roscoe, M. van Roozendaal and F. Goutail. SAOZ measurements of stratospheric NO₂ at Aberystwyth. J. Environ. Monit. 8, 353 – 361, 2006.

Instrument Description:

The SAOZ consists of a commercial Jobin-Yvon CP200 flat field spectrometer equipped with a holographic 360 gr/mm grating and a Hamamatsu 1024 diode array uncooled detector, with a 50 micron entrance slit allowing an average resolution of the order of 1 nm in the range 300-600 nm.

The spectrometer is housed in a dust- and water-proof container with a quartz window to enable measurements from the zenith sky.

The instrument is driven by a PC (with Windows 95 operating system) and records and analyses the spectra in real time. Measurements are performed from sunrise to sunset until a Solar Zenith Angle (SZA) of 94°.

The exposure time is adjusted automatically between 0.1s to 60s in order to optimise the signal and the spectra are co-added in memory during a 60s duty cycle. The dark current is measured each time the duration of exposure changes and subtracted. Averages of ozone and NO₂ morning and evening vertical columns measured between 86° to 90° SZA (91° SZA for NO₂).

Algorithm Description:

Since c. 2015 analysis is automatically carried daily using QDOAS v2.103 operated within a Matlab wrapper function that also handles file read and write for submission purposes (previously WinDOAS was used and run manually on a circa monthly basis). Historic data from 1998 have also been

reprocessed with the current algorithm and settings. QDOAS settings were chosen to align with those recommended in the NDACC UV-VIS Working Group documents "Recommendations for NO₂ column retrieval from NDACC zenith-sky UV-VIS spectrometers" v3.0 and "Recommendations for total ozone retrieval from NDACC zenith-sky UV-VIS spectrometers" v2.0.

For completeness the process is outlined here. The wavelength calibration alignment is made by reference to the Fraunhofer solar absorption lines (Kurucz 1984). Following this, measured spectra are normalised (divided) by a single reference spectrum recorded at high sun on a clear and unpolluted day. Monotonic large trends are then removed by subtracting the same spectrum smoothed at a broad bandpass resulting in an atmospheric differential spectrum, in which narrow features corresponding to absorption by ozone, nitrogen dioxide, O₄ (oxygen dimer), water vapour and OClO, are remaining.

Slant columns are then calculated by least squares fitting between the signal and the differential cross sections of each absorber in an iterative process in which the contributions of the various species are calculated and removed sequentially. Ozone is measured in the Chappuis visible bands (450-550 nm) where the cross sections are independent of the temperature; nitrogen dioxide in 425-490 nm range.

The differential cross-sections of each component species are taken from the following:

NO₂ uses the low temperature 220K reference data set of Vandaele et al. (1997)

O₃ uses the 223K Chappuis bands dataset of Bogumil et al (2003)

H₂O use the HITRAN data base

O₄ uses the wavelength-corrected absorption cross-section reference of Greenblatt et al. (1990) plus a suitable cross-section for the ring effect.

Look up tables of O₃ and NO₂ air mass factors have been produced and constructed as per the recommendation documents, with the ozone climatology being derived from 10 years' worth of local overpass data. Mean vertical columns of NO₂ and O₃ for morning and evening periods are calculated as weighted averages according to the relative error in individual retrievals.

Expected Precision/Accuracy of Instrument:

Precision given in data files. For total column, precision approximately 2 DU for ozone and 1.5 E14 mol/cm² for NO₂.

Data Quality Notes:

Data pre-May 1998 analysed using SPC analysis for Ozone, post-May 1998 originally analysed using WinDOAS. During 2015 new analysis procedure based on QDOAS v2.103 initiated with historic data (1998 onwards) re-analysed and resubmitted.

All data analysed using fitted (not prescribed) slit function.

Instrument History:

Installed at Aberystwyth (52.41N, 4.06W) March 1991.

Based at Lerwick (60N, 1W) from 2/11/91 - 9/5/92,

at Aberdeen (57N, 2W) from 8/2/94 - 3/5/94,

at Camborne (50N, 5W) from 9/9/94 - 23/9/94,
and at OHP (44N, 6E) from 8/6/96 - 21/6/96.

Original PCD 512 detector replaced in December 1992 with a NMOS 512 detector.

NMOS 512 detector replaced with NMOS 1024 detector in May 1998 at same time as changing from HP to PC control.

Moved from University of Wales Aberystwyth to a nearby field site August 2006

Instrument returned to LATMOS for repairs 2015

GPS unit reached the end of its life in May 2019. An attempt was made to fit a new one but this was unsuccessful and without it the SAOZ does not work. Without funding to effect a repair, the instrument was retired in summer 2019 and no further data will be collected.