## **Data Set Description:**

PI:	Andrea PAZMINO (Previous PI: Paul Eriksen)
	CoI: Nis Jepsen
	SAOZ UV-Visible Spectrometer
Site(s):	Søndre Strømfjord 66.99 N 50.95 W 130-300 msl
Measurement Quantities:	O3, NO2

## **Contact Information:**

Name:	Andrea PAZMINO
Address:	LATMOS UVSQ/SU/CNRS, Quartier des Garennes,
	11, Boulevard d'Alembert, 78280, Guyancourt, France
Phone:	33 (0)1 80 28 52 54
FAX:	33 (0)1 30 57 09 42
Email:	andrea.pazmino@latmos.ipsl.fr
Name:	Nis Jepsen
Address:	DMI, Lyngbyvej 100, DK-2100 Copenhagen, Denmark
Phone:	345 3915 7336
Email:	<u>nje@dmi.dk</u>

# **Reference Articles:**

- Pommereau, J.P. and F. Goutail, O3 and NO2 Ground-Based Measurements by Visible Spectrometry during Arctic Winter and Spring 1988, Geophys. Res. Lett., 891, https://doi.org/10.1029/GL015i008p00891, 1988.
- 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, <u>https://doi.org/10.1029/GL015i008p00895</u>, 1988.
- Hendrick, F., J.-P. Pommereau, F. Goutail, R. D. Evans, D. Ionov, A. Pazmino, E. Kyrö, G. Held, P. Eriksen, V. Dorokhov, M. Gil, M. Van Roozendael, NDACC/SAOZ UV-visible total ozone measurements: improved retrieval and comparison with correlative ground-based and satellite observations. Atmos. Chem. Phys., 11, 5975–5995, <u>https://doi.org/10.5194/acp-11-5975-2011</u>, 2011.
- Adams, C., Strong, K., Batchelor, R. L., Bernath, P. F., Brohede, S., Boone, C., Degenstein, D., Daffer, W. H., Drummond, J. R., Fogal, P. F., Farahani, E., Fayt, C., Fraser, A., Goutail, F., Hendrick, F., Kolonjari, F., Lindenmaier, R., Manney, G., McElroy, C. T., McLinden, C. A., Mendonca, J., Park, J.-H., Pavlovic, B., Pazmino, A., Roth, C., Savastiouk, V., Walker, K. A., Weaver, D., and Zhao, X.: Validation of ACE and OSIRIS ozone and NO<sub>2</sub> measurements using ground-based instruments at 80° N, Atmos. Meas. Tech., 5, 927-953, <u>https://doi.org/10.5194/amt-5-927-2012</u>, 2012.
- Boynard, A., D. Hurtmans, M. Koukouli, F. Goutail, J. Bureau, S. Safieddine, C. Lerot, J. Hadji-Lazaro, J.P Pommereau, A. Pazmino, Irene Zyrichidou, D. Balis, A. Barbe, S. N. Mikhailenko, D. Loyola, P. Valks, M. Van Roozendael, P.F. Coheur, and C. Clerbaux: Seven years of IASI ozone retrievals from FORLI: validation with independent total column and vertical profile measurements. Atmos. Meas. Tech., 9, 4327–4353, <u>https://doi.org/10.5194/amt-9-4327-2016</u>, 2016.
- Boynard, A., D. Hurtmans, K. Garane, F. Goutail, J. Hadji-Lazaro, M. E. Koukouli, C. Wespes, C. Vigouroux, A. Keppens, J.-P. Pommereau, A. Pazmino, D. Balis, D. Loyola, P. Valks, R. Sussmann, D. Smale, P.-F. Coheur, and C. Clerbaux. Validation of the IASI FORLI/EUMETSAT ozone products using satellite (GOME-2), ground-based (Brewer–Dobson, SAOZ, FTIR) and ozonesonde measurements, Atmos. Meas. Tech., 11, 5125-5152, <u>https://doi.org/10.5194/amt-11-5125-2018</u>, 2018.

- Garane, K., Koukouli, M.-E., Verhoelst, T., Lerot, C., Heue, K.-P., Fioletov, V., Balis, D., Bais, A., Bazureau, A., Dehn, A., Goutail, F., Granville, J., Griffin, D., Hubert, D., Keppens, A., Lambert, J.-C., Loyola, D., McLinden, C., Pazmino, A., Pommereau, J.-P., Redondas, A., Romahn, F., Valks, P., Van Roozendael, M., Xu, J., Zehner, C., Zerefos, C., and Zimmer, W.: TROPOMI/S5P total ozone column data: global ground-based validation and consistency with other satellite missions, Atmos. Meas. Tech., 12, 5263–5287, https://doi.org/10.5194/amt-12-5263-2019, 2019.
- Bognar, K., X. Zhao, K. Strong, C. D. Boone, A. E Bourassa, D. A. Degenstein, J. R. Drummond, A. Duff, F. Goutail, D. Griffin, P. S. Jeffery, E. Lutsch, G. L. Manney, C. T. McElroy, C. A. McLinden, L. F. Millán, A. Pazmino, C. E. Sioris, K. A. Walker, and J. Zou, Updated validation of ACE and OSIRIS ozone and NO2 measurements in the Arctic using groundbased instruments at Eureka, Canada, Journal of Quantitative Spectroscopy & Radiative Transfer, <u>https://doi.org/10.1016/j.jqsrt.2019.07.014</u>, 2019.
- Compernolle, S., Verhoelst, T., Pinardi, G., Granville, J., Hubert, D., Keppens, A., Niemeijer, S., Rino, B., Bais, A., Beirle, S., Boersma, F., Burrows, J. P., De Smedt, I., Eskes, H., Goutail, F., Hendrick, F., Lorente, A., Pazmino, A., Piters, A., Peters, E., Pommereau, J.-P., Remmers, J., Richter, A., van Geffen, J., Van Roozendael, M., Wagner, T., and Lambert, J.-C.: Validation of Aura-OMI QA4ECV NO<sub>2</sub> climate data records with ground-based DOAS networks: the role of measurement and comparison uncertainties, Atmos. Chem. Phys., 20, 8017–8045, <u>https://doi.org/10.5194/acp-20-8017-2020</u>, 2020.
- 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 NO<sub>2</sub>, 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, <a href="https://doi.org/10.5194/amt-13-2169-2020">https://doi.org/10.5194/amt-13-2169-2020</a>, 2020.
- Verhoelst, T., Compernolle, S., Pinardi, G., Lambert, J.-C., Eskes, H. J., Eichmann, K.-U., Fjæraa, A. M., Granville, J., Niemeijer, S., Cede, A., Tiefengraber, M., Hendrick, F., Pazmiño, A., Bais, A., Bazureau, A., Boersma, K. F., Bognar, K., Dehn, A., Donner, S., Elokhov, A., Gebetsberger, M., Goutail, F., Grutter de la Mora, M., Gruzdev, A., Gratsea, M., Hansen, G. H., Irie, H., Jepsen, N., Kanaya, Y., Karagkiozidis, D., Kivi, R., Kreher, K., Levelt, P. F., Liu, C., Müller, M., Navarro Comas, M., Piters, A. J. M., Pommereau, J.-P., Portafaix, T., Prados-Roman, C., Puentedura, O., Querel, R., Remmers, J., Richter, A., Rimmer, J., Rivera Cárdenas, C., Saavedra de Miguel, L., Sinyakov, V. P., Stremme, W., Strong, K., Van Roozendael, M., Veefkind, J. P., Wagner, T., Wittrock, F., Yela González, M., and Zehner, C.: Ground-based validation of the Copernicus Sentinel-5P TROPOMI NO<sub>2</sub> measurements with the NDACC ZSL-DOAS, MAX-DOAS and Pandonia global networks, Atmos. Meas. Tech., 14, 481–510, <u>https://doi.org/10.5194/amt-14-481-2021</u>, 2021.
- Pazmiño, A., Goutail, F., Godin-Beekmann, S., Hauchecorne, A., Pommereau, J.-P., Chipperfield, M. P., Feng, W., Lefèvre, F., Lecouffe, A., Van Roozendael, M., Jepsen, N., Hansen, G., Kivi, R., Strong, K., and Walker, K. A.: Trends in polar ozone loss since 1989: potential sign of recovery in the Arctic ozone column, Atmos. Chem. Phys., 23, 15655–15670, <u>https://doi.org/10.5194/acp-23-15655-2023</u>, 2023.

## **Recent campaigns:**

O3 and NO2: CINDI-2 (Cabauw Intercomparison campaign of Nitrogen Dioxide measuring Instruments 2), in September 2016, KNMI Cabauw/CESAR site, The Netherlands

Kreher et al., Intercomparison of NO<sub>2</sub>, O<sub>4</sub>, O<sub>3</sub> and HCHO slant column measurements by MAX-DOAS and zenith-sky UV–visible spectrometers during CINDI-2, Atmos. Meas. Tech. (2020), 13, 2169–2208, <u>https://doi.org/10.5194/amt-13-2169-2020</u>

Renew of SAOZ NDACC labellisation Labellisation of the new miniaturized version, the Mini-SAOZ.

O3 and NO2: CINDI-3 (Cabauw Intercomparison campaign of Nitrogen Dioxide measuring Instruments 2), in May-June 2024, KNMI Cabauw/CESAR site, The Netherlands

# **Instrument Description:**

The SAOZ is made of a commercial Jobin-Yvon CP200 flat field spectrometer equipped with a holographic grating and a Hamamatsu diode array uncooled detector, with an entrance slit allowing an average resolution of the order of 1 nm in the range 300-600 nm. The first version (SAOZ-512) was using a 200 gr/mm grating associated to a 512-diode array detector and a 25-micron entrance slit and the second one (SAOZ-1024) was using a 360 gr/mm grating associated to a 1024 diode array detector and a 50-micron entrance slit allowing a better oversampling (2 instead of 1). The equipment which is ran in the outside, is placed in a sealed tight and dehydrated box on the top of which a quartz window is mounted in order to look at the zenith sky with a total field of view of 10°. As SAOZ was designed to measure especially in the Polar Regions, sometimes of difficult access, the system is completely automated, maintenance is simple (mechanical shutter).

The instrument is driven by an external computer which records and analyses the spectra in real time. Measurements are performed from sunrise to sunset up to a Solar Zenith Angle (SZA) of 94°. The exposure time is adjusted automatically between 0.1s to 60s according to the light level and the spectra are co-added in memory during a 60s duty cycle. The data from a GPS device is used for SZA and time calculation. Dark current spectra are measured each time the duration of exposure changes and subtracted. Averages of ozone and NO2 morning and evening vertical columns measured between 86 and 91 SZA are calculated and transmitted in real time to the laboratory through internet. Columns transmitted to NDACC database are real time data. Every year data is reprocessed and submit to NDACC database.

## **Algorithm Description:**

## -----

A new version of processed algorithm (V3) was developed in 2013 in the frame of NORS/EU project. This is the only version available on NDACC for this station. The data processing is achieved into 3 steps:

**1. Level 0:** acquisition of the spectrum and other parameters as GPS location and temperature inside the instrument.

**2. Level 1:** Spectroscopic analysis using the DOAS technique.

- Accurate wavelength alignment using Fraunhofer solar absorption lines

- Division of the measured spectrum by a reference spectrum recorded at high sun on a clear and unpolluted day.

- Monotonic large trends are removed by subtracting the same spectrum smoothed with a broad bandpass filter (40nm) resulting in an atmospheric differential spectrum, into which narrow features corresponding to absorption by ozone, nitrogen dioxide, O4 (oxygen dimer), water vapor, and O2, are remaining.

- Calculation of slant columns 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 (450-550nm)

where the cross sections are weakly dependent of the temperature; nitrogen dioxide in 410-530nm range; O4 in 440-544nm; H2O in 500-555nm and O2 around 620nm.

3. Level 2: Conversion of slant columns into total columns using an Air Mass Factor (AMF).

- For ozone, daily AMF are calculated by UVSPEC/DISORT radiative transfer model (Mayer et Kylling, 2005). The model uses a multi-entry data-base from TOMS version 8 (TV8) ozone and temperature profiles climatology (Mc Peters et al. 2007). The TV8 is a monthly-zonal climatology sorted according to the ozone column. The parameters considered are fitting window central wavelength (510nm), station ground albedo and location (latitude, longitude, altitude), day of year, ozone slant column and SZA. The software is available on the Belgian Institute for Space Aeronomie (BIRA-IASB) web site (http://uv-vis.aeronomie.be/groundbased/)

- For NO2, daily AMF are calculated by UVSPEC/DISORT radiative transfer model. The model uses a multi-entry data-base from NO2 sunrise and sunset profiles climatology based on Satellite/SAOZ-balloon data and temperature profiles. The parameters considered are fitting window central wavelength (470nm), station ground albedo and location (latitude, longitude, altitude), day of year, time and SZA. The time of measurement is an important information since NO2 displays a large diurnal variation. The software is available on the BIRA-IASB webpage.

Vertical columns are calculated by adding the residual amount of constituent still present in the reference spectrum and divided but the corresponding AMF.

Mean twilight vertical columns are obtained by taking a weighted average of individual measurements between 86 and 91° SZA.

NO2 and O3 vertical columns are computed using the last NDACC UV-Vis recommendations (spectral windows, cross-sections, climatological AMF, ...) available on the BIRA-IASB web site.

## **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 O3SCDs. 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, an uncertainty can be quoted 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 (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. In the case of NO2, much larger errors can be obtained when tropospheric NO2 is produced or transported above the station. Such pollution events are usually easily detected by inspection of the SZA dependency of the NO2 SCDs and are filtered out in the analysis process. In summary total accuracy on vertical columns could be estimated in most cases better than 15% for NO2, and better than 5% for O3.

#### **Instrument History:**

#### -----

The SAOZ instrument was installed previously at Thule station. It was moved to Søndre Strømfjord in September 2017.

Instrument n°:	7
Period:	2017/09/12 – present
Spectrometer:	Jobin Yvon CP200, grating: 360 gr/mm, 270-600nm
Measured FWMH:	1.17nm
Detector:	NMOS, 1024 pixel
Entrance slit:	50 microns
Analysis software:	L1/L2: SAM V5.9/Igor