MetaData File provided: September 2010
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Data Set Description:

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Instrument: UV-VIS Spectrometer (two: UT-GBS and PEARL-GBS)

Site(s): Eureka, Nunavut (CANDAC PEARL facility)
NDACC Station Eureka
80.05 N, 86.42 W, 610 m above sea level

Measurement Quantities: Ozone and NO_2 vertical column densities above Eureka in units of [molecules/cm^2]

DOI: No DOI has been assigned to data archived on NDACC

DOIs for two papers using Eureka UV-VIS data:

- K. Bognar, K. Strong, R.Y.-W. Chang, P. Fogal, and P.L. Hayes. Profiles of BrO and aerosol retrieved from PEARL-GBS MAX-DOAS measurements at Eureka, Canada, https://doi.org/10.5683/SP2/GJENGJ, Scholars Portal Dataverse, V1, 2020.
- K. Bognar, R. Alwarda, K. Strong, M.P. Chipperfield, S.S. Dhomse, J.R. Drummond, W. Feng, V. Fioletov, B. Herrera, E.M. McCullough, T. Wizenberg, and X. Zhao. Replication data for: Unprecedented spring 2020 ozone depletion in the context of 20 years of measurements at Eureka, Canada, https://doi.org/10.5683/SP2/OLZ4PK, Scholars Portal Dataverse, V1, 2020.

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Instrument Description:

The PEARL ground-based spectrometer (PEARL-GBS) and the University of Toronto GBS (UT-GBS) are both Triax-180 spectrometers, built by Instruments S.A. (ISA)/Jobin Yvon Horiba, with slight differences in their slits, gratings, charge coupled device (CCD) detectors, and input optics. Both have been operated at Eureka, Nunavut, Canada (80.05N, 86.42W), in the building first known as the Arctic Stratospheric Ozone Laboratory (AStrO, operated by Environment Canada) and later renamed the Polar Environment Atmospheric Research Laboratory (PEARL) Ridge Lab, operated by the Canadian Network for the Detection of Atmospheric Change (CANDAC) from 2005 onwards.

The UT-GBS was assembled in 1998 for the MANTRA balloon campaigns, and was deployed to make measurements at AStrO/PEARL Ridge Lab during polar sunrise from 1999-2001 (Bassford et al., 2000; Farahani, 2006; Melo et al., 2004) and 2003-2011 (Fraser, 2008; Fraser et al., 2008, 2009). Furthermore, the UT-GBS took summer and fall measurements at the PEARL Ridge Lab in 2008 and from 2010 onwards. For 1999-2001, the UT-GBS was installed outside in a temperature-controlled aluminum case, while for 2003-2017, it was installed inside a viewing hatch. In 2015, a sun-tracker was installed above the instrument to allow MAX-DOAS measurements. The PEARL- GBS was assembled and permanently installed inside a viewing hatch in the PEARL Ridge Lab in August 2006 and has been taking measurements during the sunlit part of the year since then (Adams et al., 2010; Adams, 2012; Fraser, 2008; Fraser et al., 2009). In March 2008, a sun-tracker was installed above the instrument to allow for direct-sun and MAX-DOAS measurements. From 2006 to 2010, the PEARL- GBS focused on zenith-sky measurements in the visible range. Since 2011, the PEARL-GBS is focused on MAX-DOAS measurements in the UV, with BrO as the main target species.

The GBSs have similar input optics with a field-of-view of 2 degrees. They both have three gratings, which are attached to a motorized turret. Resolution varies across the CCD chip from 0.5-2.5 nm for ozone; 0.5-1.0 nm for NO2 retrieved in the visible region (NO2-vis); and 0.2-1.0 nm for NO2 retrieved in the UV region (NO2-UV). Spectra from the GBSs are recorded using thermoelectrically cooled back-illuminated CCD detectors manufactured by ISA. The original UT-GBS CCD, used from 1999-2004, had 2000x800 pixels and reached temperatures of 230-250 K (Bassford et al., 2000). From 2005 onwards, a 2048x512 pixel CCD, which operated at a temperature of 201-205 K, was used for the UT-GBS. The PEARL-GBS CCD is identical to the UT-GBS CCD, except it is coated with an enhanced broadband coating and its operating temperature oscillates slightly from 203-205K on timescales of approximately 5 min.

The UT-GBS has three gratings, listed below, with different resolutions. Note that changes to the instrument input optics in 2012 reduced aberrations and improved the signal level.

UT-GBS Grating (gr/mm)	Res. 1998-2004 (nm) Original setup	Res. 2005-2009 (nm) New CCD	Res. 2010 (nm) New CCD + input optics	Res. 2011 (nm)	Res. 2012-2023 (nm) New CCD + new input optics

				New CCD + input optics + new fibre	
400	0.8-5.4	0.8-5.4	1.1-2.1	0.9-1.4	0.5-2.3
600	0.5-2.3	0.5-2.3	0.9-1.3	0.6-2.0	0.4-2.3
1800	0.2-0.8	0.2-0.8	0.2-0.3	0.2-0.3	0.1-0.4

The PEARL-GBS has three gratings, listed below, with different resolutions. Note that changes to the instrument input optics in 2010 reduced aberrations and improved the resolution. The flat CCD mount replaced with wedged one in 2013 for improved uniform resolution.

PEARL-GBS Grating (gr/mm)	Res. 2006-2009 (nm) Original setup	Res. 2010 (nm) New fibre	Res. 2011-2012 (nm) New fibre + slit	Res. 2013-2023 (nm) New fibre + slit + wedged CCD mount
300	1.0-3.0	0.9-1.3	1.4-3.0	1.4-3.7
600	0.5-2.5	0.4-0.6	0.7-1.5	0.7-1.5
1200	0.2-1.8	0.17-0.19	0.3-0.5	0.3-0.5

Measurement History:

Note: “year-round” measurements are made from polar sunrise in mid-February to polar sunset in mid-October.

UT-GBS

- 1999: spring measurements only, 300 gr/mm grating.
- 2000: spring measurements only, 600 gr/mm grating.
- 2001: NO DATA, mechanical slit jammed open, resolution dramatically reduced.
- 2002: NO DATA, the instrument was not in Eureka for 2002.
- 2003: data acquisition error, reduced SNR. 300+600 gr/mm gratings.
- 2004: data acquisition error, reduced SNR. 300 gr/mm grating.
- 2005: spring measurements only, 600 gr/mm grating.
- 2006: spring measurements only, 600 gr/mm grating.
- 2007: spring measurements only, 600 gr/mm grating.
- 2008: spring measurements only (UV measurements for the rest of the year), 600 gr/mm grating.
- 2009: spring measurements only (instrument participated in the CINDI campaign in the Netherlands in the fall), 600 gr/mm grating.
- 2010: year-round, 600 gr/mm grating.
- 2011: year-round, 600 gr/mm grating.
- 2012: spring measurements only, summer/fall data lost due to lack of on-site support and instrument overheating. 600 gr/mm grating.
- 2013: year-round, 600 gr/mm grating.
- 2014: year-round, 600 gr/mm grating.
- 2015: year-round, summer data lost due to CCD gain issue. 600 gr/mm grating.

- 2016: year-round, summer data lost due to CCD gain issue. 600 gr/mm grating.
- 2017-2023: year-round, 600 gr/mm grating (some data gaps due to power outages, instrument issues, and reduced on-site support during and after the pandemic).

PEARL-GBS

- 2006: Fall data only, 600 gr/mm grating.
- 2007: spring + second half of the year (UV measurements in first half), 600 gr/mm grating.
- 2008: spring + second half of the year (UV measurements in first half), 600 gr/mm grating.
- 2009: second half of the year (UV measurements in first half), 600 gr/mm grating.
- 2010: second half of the year (UV measurements in first half), 600 gr/mm grating.
- 2011-2023: UV measurements only, 1200 gr/mm grating (some data gaps due to power outages, instrument issues, and reduced on-site support during and after the pandemic).

Algorithm Description:

July 2018 (Version 002 and Version 003)

IMPORTANT: Version 2 is assigned to CAMS Rapid Delivery data, while version 3 indicates consolidated archived data. The versions 2/3 processing is identical, with the exception of the inputs to the ozone AMF look-up tables. The version 3 ozone product uses ozonesonde total columns as AMF LUT input. Ozonesonde data are not available in time for rapid delivery, and so version 2 ozone uses a two-step approach: AMF LUT inputs are fixed at 300 DU in the first step, and the VCDs from the first step are used as AMf LUT input for the final VCDs. Radiosonde T and P profiles might also be replaced by standard atmosphere in v2 files, depending on data availability. The v2/3 NO2 products are identical.

The main issue corrected in v2/3 concerns the VCD calculation in version 1. Due to a coding error, the lower confidence bound of the RCD was used in the VCD calculations, instead of the actual RCD value given by the Langley plots. This issue affects all the VCDs in version 1, and is fixed in v2/3.

Further changes in v2/3 compared to v1:

The NO2 retrievals now use the NDACC-recommended 425-490 nm wavelength range.

The systematic residuals were noticed for PEARL-GBS NO2 retrievals, so a residual cross-section was created and included in the fit following the methods outlined below. The NO2 DSCDs did not require the correction that was needed for the ozone DSCDs. Systematic residuals were not apparent in the UT- GBS NO2 fits.

For all other detail on the algorithm, see the description below. The error filters applied to the dataset are described under the �Expected Precision/Accuracy of Instrument� section.

October 2017 (Version 001)

Data were analyzed for zenith-sky, multi-grating measurements, using the methods recommended by the NDACC UV-Vis Working Group. Gaps in data submitted to the archive occur when the instrument was taking UV measurements for BrO, and for some periods, particularly near summer solstice, when DOAS residuals had large systematic errors.

DSCDs were calculated using the QDOAS software. DOAS fits were performed with a 3rd order polynomial in the 450-545 nm region for ozone, and the 425-450 nm region for NO2. O3 at 223 K (Bogomil et al, 2003), NO2 at 220 K (Vandaele et al, 1997), H2O (HITRAN, 2004), corrected O4 (Greenblatt et al, 1990), and Ring (Chance and Spurr, 1997) cross-sections were all fit to the data. Daily reference spectra were used for the QDOAS analysis.

For both the UT-GBS and PEARL-GBS, intermittent systematic residuals appeared in the DOAS ozone fits. In order to characterize and correct for these residuals, they were smoothed using running averages and included as cross-sections in the ozone DOAS analysis. These residual cross-sections were fit in the ozone retrievals for the 600 gr/mm UT-GBS and PEARL-GBS time-series up to and including 2017 (note that the 300/400 gr/mm measurements did not need this cross-section). The magnitude of the systematic residuals was much larger for the PEARL-GBS than for the UT-GBS. The PEARL-GBS DSCDs showed a correlation with the magnitude of the residuals, so the DSCD values were corrected with the slope of this correlation. Details may be found in Cristen Adams' PhD thesis (see below). No such correction was necessary for the UT-GBS data. After changes to the optical setup of the instruments (in 2012 for the UT-GBS and in 2013 for the PEARL-GBS), the systematic residuals have been greatly reduced or eliminated. Note that the PEARL-GBS took no visible measurements after 2010.

Vertical column densities (VCDs) were calculated using the Langley method. Reference column densities (RCDs) were calculated using Langley plot in the SZA=86-91 range, or the nearest available 5 degree range in the summer. In the spring when the SZA values are still over 86 degrees, the max. allowed SZA was set to 92 degrees. RCDs were calculated for each twilight, and the two values were averaged to get a more accurate daily RCD value.
VCDs for each SZA over the twilight were then calculated using VCD = (DSCD + RCD) / AMF.

The twilight VCDs were calculated using weighted average formulae in the selected SZA range. The weight of each VCD was estimated as the DSCD fitting error divided by the AMF.

Ancillary Data:

July 2018 (version 2/3): No changes compared to v1.

October 2017 (version 1):

Cross-sections: O3 at 223 K (Bogomil et al, 2003), NO2 at 220 K (Vandaele et al, 1997), H2O (HITRAN, 2004), corrected O4 (Greenblatt et al, 1990), and Ring (Chance and Spurr, 1997)

Ozone AMFs: NDACC look-up table air-mass factors (AMFs) V2_0

NO2 AMFs: NDACC look-up table air-mass factors (AMFs) V1_0

Ozonesonde profiles: sonde total columns interpolated to the measurement times were used as the input for the ozone AMF look-up table (see Algorithm Description). Ozonesondes are launched from Eureka Weather Station on a weekly basis.

<u>Expected Precision/Accuracy of Instrument:</u>

<u>July 2018 (version 2/3):</u>

Random errors are calculated according to the following table:

Error	Multiply by	Multiplication factor for Ozone	Multiplication factor for NO2
Instrument error	SCD	0.01	0.01
Line filling by Raman scattering	SCD	0.01	0.05
QDOAS fitting errors	QDOAS error	3	3
Systematic residual	residual DSCD	1e17 mol/cm2	N/A
AMF error	AMF	0.0364	0.05

In addition, the 1-sigma standard deviation of the VCD(SZA) over the given twilight was added to the random error in quadrature.

Systematic errors are calculated according to the following table:

Error	Multiply by	Multiplication factor for Ozone	Multiplication factor for NO2
Absolute cross-section	SCD	0.031	0.05
Cross-section T-dependence	SCD	N/A	0.08
RCD baseline error	N/A	1e17 mol/cm2	2e15 mol/cm2
RCD variation	|RCD_am-RCD_pm|	0.5	0.5

The total error is calculated as the root mean sum of the systematic and random errors.

The error filters applied to the dataset were as follows:

Parameter	Ozone filter	NO2 filter
Total error	<60 DU	<2e15 mol/cm2 or <200%
Langley plot R^2	>=0.9 (0.8 for 2003-04)	>=0.6
Min. accepted SZA range	2 degrees	2 degrees
Min n.o. points in Langley	8	8

In addition, NO2 measurements were only accepted if both morning and evening twilights were available, in order to avoid biased RCD values caused by the diurnal variation of NO2 in the spring. For ozone, when one twilight was missing, the RCD error (and therefore the systematic error) could not be calculated. In those cases, when the other twilight passed all other error filters, the systematic error was interpolated from the nearest two valid measurements.

Data were also filtered to ensure that >50% of data points pass the CAMS error filters.

<u>October 2017 (version 1):</u>

Random Errors are the 1-sigma standard deviation of the VCD(SZA) over the given twilight.

Systematic Errors were calculated through error tables which may be found in Cristen Adams' PhD thesis.

Error in Weighted Mean is primarily used as a diagnostic (if the value is large, something went wrong in the retrievals). For each VCD(SZA) over a given twilight, a rough estimate of error is calculated as ERR(SZA) = DSCD(SZA)/AMF(SZA). Then a twilight VCD was calculated by taking the weighted mean of VCD(SZA), weighted by ERR(SZA).

The Total Error is calculated as the root mean sum of the systematic and random errors.

<u>Instrument History:</u>

<u>UT-GBS</u>

- 1998: Assembly.
- 1999: First spring campaign to Eureka.
- 2005: The original CCD detector (back-illuminated chip, with 2000x800 pixels) was replaced with a new CCD (2048x512 pixels).
- March 2011: Liquid light guide replaced with a 1-m slit-to-spot fibre bundle.
- March 2012: Mechanical slit and F/# matcher were replaced with fixed slit and AFO-XY fiber mount. February 2013: 1-m spot-to-slit fibre bundle replaced with a 10-m one
- March 2015: Sun-tracker installed, instrument placed in air-conditioned box

<u>PEARL-GBS</u>

- August 2006: Installation.
- March 2008: Sun-tracker installed above instrument. March 2009: Light-leaks to instrument corrected.
- March 2010: Liquid light-guide replaced with a spot-to-slit fiber bundle (for improved resolution).

- March 2013: The 1-meter spot-to-slit fiber bundle was replaced with 6-meter one. The flat CCD mount was replaced with a wedged one (for improved uniform resolution).
- October 2014: Sun-tracker moved to better position on the roof of the Ridge Lab, 6-m spot-to-slit fibre bundle replaced with a 30-m one
- March 2017: Instrument placed in air-conditioned box

Reference Articles:

PhD Theses

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Selected Articles
For a complete list, see: http://www.atmosp.physics.utoronto.ca/people/strong/papers.html

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