New Total Column Ozone and Trace Gas Measurements from the Pandora Spectrometer System

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Introduction

Ozone (O_3) is a critical atmospheric constituent that is involved in the photochemistry of both the troposphere and stratosphere. *Frequent measurements of O_3 total column amounts and vertical distribution are essential for quantifying the role of tropospheric O_3 in local and regional environmental degradation, tropospheric chemistry, surface UV-B levels, human health, and radiative forcing.*

We present new measurements of total column ozone, TCO, derived from ground-based direct solar irradiance measurements using our recently developed Pandora single grating spectrometer system. Ozone retrievals were performed using a DOAS spectral fitting algorithm (310-330 nm) after correction for stray light effects. *The high spectral resolution Kurucz [2005] extraterrestrial spectrum, normalized to SUSIM, and convoluted with the Pandora slit function, was used as a reference for determining O_3 amounts.*

Pandora high temporal resolution TCO measurements (every 5 sec) are presented for two moderately polluted sites in the US: GSFC (Goddard Space Flight Center), in Maryland, and Langley, in Virginia. Data are also shown from our CINDI campaign in Cabauw, Netherlands (June-July 2009). Comparisons between Pandora, a standard ozone network double-grating Brewer spectrometer (#171), and Aura-OMI (Ozone Measuring Instrument) satellite data are discussed.

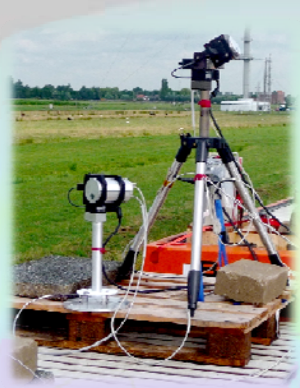

Figure 1: Sky-radiance plus direct-sun Pandora (center) and direct-sun only Pandora (right) in Cabauw.

Methods

The **Pandora CCD spectrometer system** consists of an Avantes fiber optic spectrometer with a UV sensitive back-thinned 2048x16 pixel CCD coupled to an optical head with two 9-position filter-wheels (Open, Opaque, 280-320 nm bandpass, 280-380 nm bandpass, Polarizer-1 Polarizer-2, Polarizer-3, and four neutral density filters). The **Pandora CMOS system** has 1024 pixels and one 9-position filter-wheel (Table 1). The optical head is connected to an electronics control box and is mounted on a computer controlled sun-tracker and sky-scanner (~0.01° pointing precision).

Calibration-Stability: The spectrometer is temperature stabilized inside of a small enclosure to ensure measurement stability. Wavelength calibration and the slit function are determined from lamp emission lines (Hg, Cd, Cu, In, Mg, Zn), several laser lines from 325 nm to 532nm. Wavelength stability is validated by an analysis of the solar Fraunhofer line structures.

Stray-Light: Two UV bandpass filters (280-320 and 280-380 nm with sharp cutoffs at 320 and 380 nm, respectively) are used to greatly reduce stray light (< 10^{-5}) at short wavelengths (290-320nm).

Total column: For total column (TC) trace gas amounts (Tables 2, 3) Pandora is operated in direct-sun viewing mode using a solar tracker and a sun-centroiding algorithm. Retrievals are performed using a direct-sun DOAS (Differential Optical Absorption Spectroscopy) spectral fitting algorithm and laboratory measured cross sections. The fitted functions are a low-order polynomial, the absorption spectra of each atmospheric absorber, and wavelength shift and squeeze functions [Herman et al., 2009]. The independently measured Kurucz [2005] extraterrestrial spectrum, convoluted with the Pandora slit function, is used as a reference for O_3 and NO_2 retrievals.

Vertical distributions of O_3 and NO_2: can be retrieved from multiple angle views of sky radiance (Table 2).

Table 1: Characteristics

Wavelength interval (nm)	280-530
Spectral resolution (FWHM)	0.5nm
Oversampling	~ 2 pixels
CMOS (pixels)	1024x1
Direct-Sun FOV	1.6°
Pointing Precision	0.01°

Table 2: Pandora capabilities

Mode	Resp.	Parameter	Precision	Uncertainty
Pandora Direct-Sun	4 sec	Total Column O3, NO2, SO2, H2O, HCHO, CHOCHO	0.01 DU	0.1 DU
Pandora Sun-Sky	10 min	O3 profile (3-5 km res)	1 DU	height dep.
	10 min	NO2 profile (1 km res)	0.01 DU	height dep.

Table 3: Characteristics of the various TC retrieval algorithms

Trace gas	Fitting window	Cross sections	Calibration method
O_3	310-330nm	Bass and Paur [1985] at 225K	Use Extraterrestrial spectrum
NO_2	400-460nm	Vandaele et al. [1998] at 255K	Use Extraterrestrial spectrum
SO_2	310-330nm	Vandaele et al. [1994] at 259K	MLE (modified Langley extrap.)
H_2O	464-515nm	Rothman [2009] at 273K	MLE
HCHO	328-357nm	Meller and Moortgat [2000] at 257K	MLE
CHOCHO	414-457nm	Volkhamer et al. [2005] at 257K	MLE

Pandora and Brewer Ozone

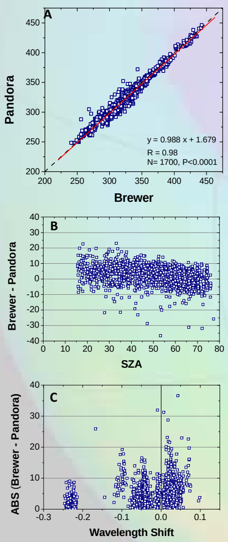

Figure 2A: Comparison between TCO measurements from Pandora and the Brewer double-grating spectro-meter (#171), collocated at the GSFC site. Pandora data were interpolated to the Brewer time (only if closer than 5 minutes). Pandora measurements were filtered for Normalized RMS of weighted spectral fitting residuals < 0.05, and uncertainty in TCO <2 DU. Brewer measurements were filtered for standard error in TCO < 2 DU.

Figure 2B: TCO difference between Brewer and Pandora as a function of Solar Zenith Angle (SZA).

Figure 2C: Absolute difference in TCO between Brewer and Pandora as a function of Wavelength Shift (due to changes in temperature). A shift of 0.24 nm is the same as the spectral distance between pixels on the Pandora CMOS detector (250 nm/1024 pixels) .

Pandora and Aura-OMI Ozone

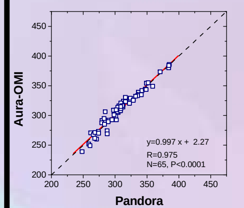

Figure 3: Comparison between Pandora TCO and Aura-OMI (GSFC overpass, ovpid: 447, OMTO3 v8.5, Collection 3; http://avdc.gsfc.nasa.gov). Pandora data were averaged over a ± 1-hour window of the OMI overpass. Pandora measurements were filtered for Normalized RMS of weighted spectral fitting residuals < 0.05, and uncertainty in TCO <2 DU. OMI data were filtered for distance < 50 km and Cloud-fraction < 0.2.

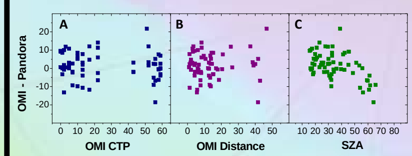

Figure 4: Difference in total column ozone amounts (in DU) measured by OMI and Pandora as a function of: (A) OMI Cross Track Position (CTP, in the range 0-59); (B) OMI distance from GSFC location (in the range 0-50 km, due to the filtering we applied to the OMI data); (C) Solar Zenith Angle (SZA, from OMI).

Pandora Ozone time series at GSFC, Cabauw and Langley

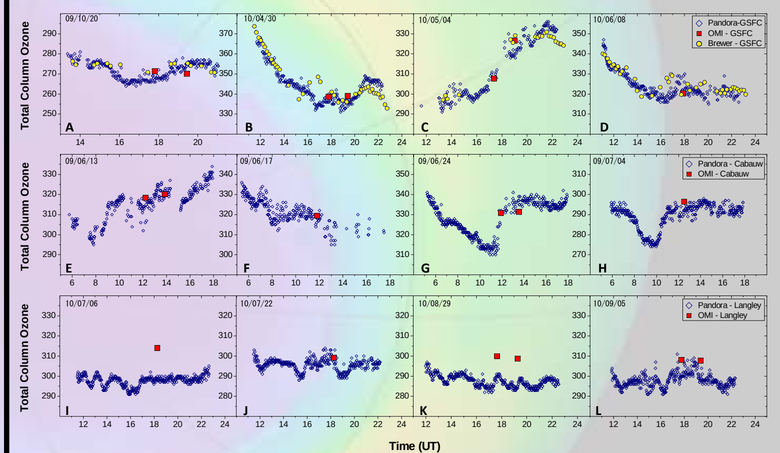

Figure 5: Time series of Aura-OMI and Pandora Total Column ozone (TCO) data measured at: **(A)-(D)** the GSFC site, MD (Pandora-9 data, available since 26 May 2009); **(E)-(H)** Cabauw, Netherlands (Pandora 9 data, CINDI campaign during 9 June-20 July 2009); and **(I)-(L)** Langley, VA, (Pandora 6 data, available since 24 June 2010). Measurements of TCO made by the collocated Brewer instrument are also shown for GSFC. Close agreement between OMI and Pandora was consistently observed at GSFC (R=0.975) and Cabauw (R=0.962), with average difference between OMI and Pandora of 1.5 DU and 2.5 DU, respectively. In most cases OMI overestimated TCO at the Langley site (average difference between OMI and Pandora of 12.4 DU, R=0.948).

Conclusions

- Pandora and Brewer measurements at the GSFC site were found to be in close agreement throughout the day, including near sunrise and sunset conditions with solar zenith angles up to 80° (Figures 2A. 2B).
- The successful inter-comparison of Pandora and Brewer shows that the Pandora direct-sun DOAS technique can be used for validation of satellite (e.g., Aura-OMI and NPP-OMPS) retrievals of TCO.
- Pandora and Aura-OMI TCO observations over GSFC were found to be in very good agreement (R=0.975 , slope=0.997, offset=2.27 DU with OMI slightly overestimating TCO) when the OMI cross track position was at a distance of less than 50 km from the GSFC site, and OMI-measured cloud fraction was less than 0.2 (Figures 3,4).
- Close agreement was also observed at Cabauw and Langley (R=0.962 and R=0.948, respectively), although the average difference between OMI and Pandora at Langley was 12.4 DU with OMI overestimating TCO. Average difference between OMI and Pandora at Cabauw was 2.5 DU (Figure 5).
- Should be highlighted that the Pandora TCO retrievals were performed using an independently measured reference spectrum (Kurucz extraterrestrial spectrum, normalized to SUSIM, convoluted with the Pandora slit function).
- Since direct-sun measurements can be made by Pandora in the presence of light to moderate clouds, a nearly continuous record can be obtained, which is important when matching overpass times for satellite data validation.
- Considerable temporal (day-to-day and diurnal) variability was observed in TCO measured by Pandora at all three study sites: GSFC, Langley and Cabauw. Diurnal variability as high as 40 DU was observed in some cases (Figure 5). These short-term (e.g. hourly) temporal changes in ozone amounts cannot be captured by OMI or other satellite instruments in sun-synchronous orbits (daily overpass).
- Measurements of trace gas variability from our new network of Pandora spectrometers at 3 locations (soon to be 14) provide a unique dataset for testing and validating model photochemistry and capturing short-term, small-scale variability in atmospheric composition. The data from 14 sites will be particularly useful for measuring satellite sub-pixel and pixel-to-pixel variability, and validating satellite (e.g. Aura-OMI, NPP/OMPS) data so that they can be used for monitoring the response of the ozone layer to atmospheric changes and studying impacts on climate and air quality.