LuftBlick report 2021002

Quality Assurance for Earth Observation - QA4EO

WP2322 - TN on Pandora Lunar data processing set-up

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1 Summary and Conclusions

The D-3 “Pandora Lunar data processing set-up” of WP2322 of the ESA project “Quality Assurance for Earth Observation” (QA4EO) [AD1] has the goal to prototype trace gas retrievals using direct moon observations. A brief summary and conclusion of this deliverable are given in the following.

Lunar trace gas column prototypes have been developed for the gases NO_2, O_3, NO_3 and H_2O. As an initial step (phase 1 of the WP) the moon retrievals were based on direct sun reference spectra. This approach is justified in section 3. It has to be noted that only NO_2 and O_3 direct sun column products exist and consequently direct sun products for NO_3 and H_2O had to be developed first. The detailed retrieval settings, their explanation and test applications on Pandora instruments located in Rome, can be found in section 4.

NO_2 total columns: NO_2 column retrievals from lunar observations are very robust and use exactly the same fitting setup as for direct sun retrievals. Due to the elaborate AMF treatment (see [RD1]), also the transition between day and night can be nicely resolved. Due to the significantly reduced input irradiance, data averaging for lunar data is suggested (~1h).

O3 total columns: For lunar O3 columns a completely different fitting setup was needed compared to direct sun retrievals. Whilst direct sun O3 retrievals are done in the UV using a stray light blocking bandpass filter, this is not feasible for lunar observations for sake of signal strength. As a consequence, lunar gas columns are retrieved from the Chappuis band where the signal is comparably high and at the same time spectral stray light is low. Still data averaging for lunar data is suggested (~1h).

NO3 total columns: A NO3 column retrieval for direct sun observations had to be developed first. Also here the same fitting setup could be applied on sun and moon observations.

H2O total columns: Similar to NO3, a H2O column retrieval for direct sun observations had to be developed first. For the prototype we have selected the 505 nm band for the retrieval, which yields very robust H2O columns from both sun and moon observations. Extraordinary good agreement to AERONET data could be found.

Overall we see very encouraging results regarding the retrieval of lunar trace gas columns. As could be expected, the reduced signal turned out to be the strongest impact factor, mostly affecting O3 column retrievals. In future studies we will try to estimate the potential limitation in using a solar reference instead of a proper lunar reference or a lunar model.

2 Document logistics

2.1 Acronyms and Abbreviations

AD	Applicable Document
BrO	Bromide Oxide
D	Deliverable
I2	Molecular Iodine
H2O	Water Vapor
HCHO	Formaldehyde
HONO	Nitrous Acid
NO2	Nitrogen Dioxide
NO3	Nitrate Radical
O2	Molecular Oxygen
O2O2	Oxygen Dimer
O3	Ozone
OFFS	Offset Polynomial
OIO	Iodine Dioxide
PGN	Pandonia Global Network
QA4EO	Quality Assurance Framework for Earth Observation
RD	Reference Document
Rome-SAP	Sapienza University, Rome
SMO	Smoothing Polynomial
WLC	Wavelength Change Polynomial

2.2 Applicable Documents

[AD1] Quality Assurance for Earth Observation project [Annex B, Statement of Work for LuftBlick], SERCO Contract QA4EO/SER/SUB/04, 2020.

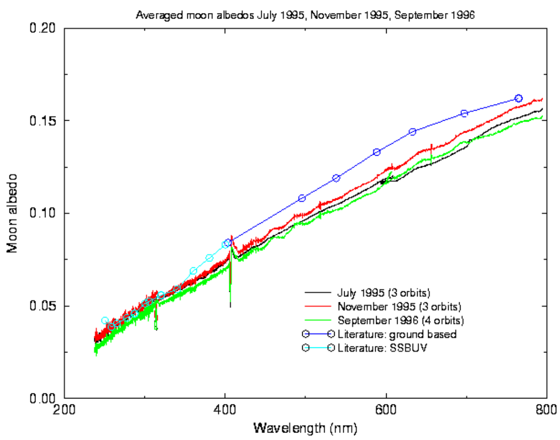
2.3 Reference Documents

[RD1] A. Cede, M. Tiefengraber, M. Gebetsberger, and E. Spinei Lind. Pandonia Global Network Data Products README Document, 2020.

[RD2] H.H. Kieffer, T. C. Stone, The spectral irradiance of the moon. Astron.J. 129, 2887–2901, 2005.

3 Lunar trace gas retrieval approach

The brightness of the lunar disc changes in a complex way not only along the moons phase angle, but also along the night. This additional complexity needs to be properly addressed in the retrieval scheme. Commonly, lunar reflectance models (like ROLO [RD2]) are applied to adjust the reference value accordingly. Retrieval schemes based on hyperspectral measurement systems usually allow a larger number of retrieval parameters which enables the inclusion of closure polynomials in the minimization. Assuming a rather smooth spectral variation of the lunar albedo, we hypothesize that sufficiently high order closure polynomials are capable of compensating for the change in the lunar spectral irradiance. As can be revealed from the figure on the left, this assumption should hold. This figure shows data from Dobber [1998] where the lunar albedo as retrieved from several sensors has been investigated.



The spectral fitting algorithm applied to Pandora data makes use of a reference spectrum taken from solar measurements. Following the above outlined hypothesis, the same solar reference spectrum is also used for the retrieval of trace gas columns from lunar measurements.

Since the spectral background only changes in a smooth way, there is no need to change anything of the fitting setup for the lunar retrievals. Hence the same setup as used for the solar retrievals is used as first guess for each lunar trace gas product.

4 Lunar trace gas prototypes

4.1 Test location and time period

For lunar trace gas prototype testing we focus on datasets collected at Rome, Sapienza university (PGN location name: Rome-SAP), between 1st and 10th of September, 2019. At that time, Pandora 117 and 138 had been on site. All time series below refer to this period and instruments.

4.2 Processing settings description

The following descriptions are adapted from the PGN product readme file [RD1].

4.2.1 Absorption cross sections

Name	Source

BrO	David M Wilmouth, Thomas F Hanisco, Neil M Donahue, and James G Anderson. Fourier transform ultraviolet spectroscopy of the 23/2? x 23/2 transition of BrO. The Journal of Physical Chemistry A, 103(45):8935–8945, 1999.
H2O, O2	Laurence S Rothman, Iouli E Gordon, Yury Babikov, Alain Barbe, D Chris Benner, Peter F Bernath, Manfred Birk, Luca Bizzocchi, Vincent Boudon, Linda R Brown, et al. The hitran2012 molecular spectroscopic database. Journal of Quantitative Spectroscopy and Radiative Transfer, 130:4–50, 2013.
HCHO	Richard Meller and Geert K Moortgat. Temperature dependence of the absorption cross sections of formaldehyde between 223 and 323 k in the wavelength range 225–375 nm. Journal of Geophysical Research: Atmospheres (1984– 2012), 105(D6):7089–7101, 2000.
HONO	J Stutz, ES Kim, U Platt, P Bruno, C Perrino, and A Febo. Uv-visible absorption cross sections of nitrous acid. Journal of Geophysical Research: Atmospheres (1984–2012), 105(D11):14585–14592, 2000.
I2	A Saiz-Lopez, RW Saunders, DM Joseph, SH Ashworth, and JMC Plane. Absolute absorption cross-section and photolysis rate of i 2. Atmospheric Chemistry and Physics, 4(5):1443–1450, 2004.
NO2	Ann Carine Vandaele, Christian Hermans, and Sophie Fally. Fourier transform measurements of so2 absorption cross sections: Ii.: Temperature dependence in the 29 000–44 000 cm- 1 (227–345 nm) region. Journal of Quantitative Spectroscopy and Radiative Transfer, 110(18):2115–2126, 2009.
NO3	Stanley P Sander. Temperature dependence of the nitrogen trioxide absorption spectrum. The Journal of Physical Chemistry, 90(17):4135–4142, 1986.
O2O2	Ryan Thalman and Rainer Volkamer. Temperature dependent absorption cross-sections of o 2–o 2 collision pairs between 340 and 630 nm and at atmospherically relevant pressure. Physical chemistry chemical physics, 15(37): 15371–15381, 2013.
O3	A. Serdyuchenko, V. Gorshelev, M. Weber, W. Chehade, and J. P. Burrows. High spectral resolution ozone absorption cross-sections - Part 2: Temperature dependence. Atmospheric Measurement Techniques Discussions, 6:6613– 6643, July 2013. doi: 10.5194/amtd-6-6613-2013. → shifted by + 3pm!
OIO	Peter Spietz. Absorption Cross Sections for Iodine Species of Relevance to the Photolysis of Mixtures of I2 and O3 and for the Atmosphere. PhD thesis, University of Bremen, 2005.

4.2.2 Retrieval parameters

Parameter	**Description**
Filters used	Pandora uses a filter wheel, where different spectral filters can be placed, specifically a U340 and a BP300 filter. U340 is a colored glass bandpass filter with peak transmission at 340 nm. BP300 is an interference bandpass filter with peak transmission at 300 nm. If none of these spectral filters is in place, the measurement

	is called OPEN. Note that direct lunar observations do not use a diffuser, while direct sun measurements do. This setting indicates, on which type of filter settings the respective r-code is applied.
Effective height	This (comma-separated) string is only used for observation modes "Direct sun" or "Direct moon" and gives the assumed effective heights for each output trace gas used to calculate the direct air mass factor (AMF, see section 4.1). For observation mode "MAXDOAS" it is not given. Each sub-string is either a value in km or a string representing a profile type from a climatology. The options for the climatology are listed in section "Climatologies" of the ATBD. The string can be followed by an uncertainty estimation in round parenthesis. This estimation can be a value in km or a string representing a profile type. E.g. "O3(2.4)" would mean the effective height is taken from the ozone climatology and its uncertainty is 2.4 km. If the uncertainty estimation is not given and a string representing a profile type is set for the effective height, then the uncertainty estimation is taken from the same climatology too, i.e. "O3" has the same effect as "O3(O3)". If the uncertainty estimation is not given and a value in km is set for the effective height, the retrieval uses half of the effective height as uncertainty, i.e. "7.2" has the same effect as "7.2(3.6)". Sub-strings can also be combined using "+" for the direct sun or moon observation mode, e.g. "BL+STRAT". In this case different effective height-estimations are used to get the best estimation of the AMF.
Number of fitting windows	This is either 1 or 2. In the latter case 2 separate fitting processes are performed and the final output data are a combination of the results of both of them (see ATBD, section "L2 Direct Algorithm"). In this case the remaining entries of the table can be strings separated by a semicolon, but only if the 2 fitting processes use different settings. The 2nd part of the string, after the semicolon, is then written in italic for easier distinction.
Reference	Synthetic reference spectrum: a spectrum, which is usually the average over several spectra measured by the Pandora unit and corrected for the estimated total optical depth from the different atmospheric extinction processes included in it. The uncertainty in these estimated optical depths, which are determined during the instrument calibration, is the driver for the common uncertainty of the product. Typically the calibration works better at stations, which are not always polluted, and consequently works worse at continuously polluted places such as large cities, which is then reflected in the common uncertainty output.
Wavelength window	The lower and upper limits of the wavelength window(s) used in the spectral fitting in nanometer [nm].
Order of polynomials	The orders of the smoothing polynomial, "SMO", offset polynomial, "OFFS", and wavelength change polynomial, "WLC" used in the spectral fitting (see ATBD, section "L2Fit Algorithm - Spectral Fitting"). E.g. "SMO 4, OFFS 0, WLC 1" means a 4th order smoothing, 0 order offset and first order wavelength change polynomial have been used. A value of "-1" means that the respective polynomial is not used in the fitting.
Fitted gases	A comma separated string listing the trace gases used in the spectral fitting, the source of the cross sections and the treatment of the temperature. Each substring has the format "GGG (TTT)". GGG refers to an entry of table 1, which lists the source of the cross sections for the respective trace gas. TTT describes the temperature treatment and can be:

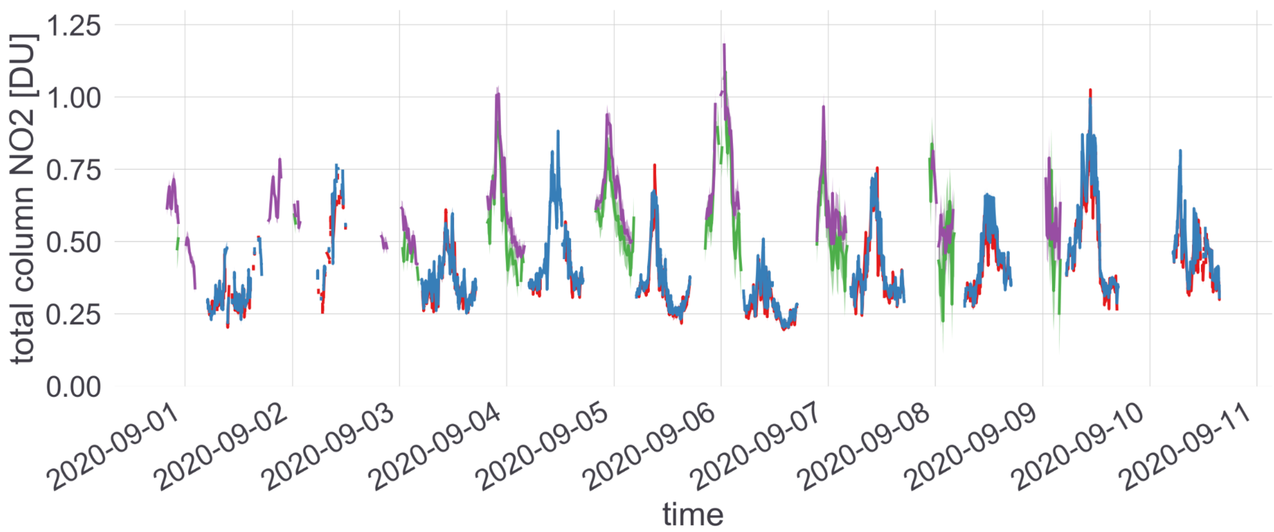
	• "T-fit": the effective temperature is fitted. • A temperature value: this means the cross sections at this fixed temperature (e.g. 225.0 K) are used in the fitting. • "XX-clim": the spectral fitting uses the temperature from climatology "XX" (see ATBD, section "Climatologies"). E.g. "O3-clim" means the effective ozone temperature climatology is used.
Molecular scattering	This is "Subtracted", if the molecular scattering cross sections [9, 17] have been subtracted before the spectral fitting, and "Not subtracted" otherwise.

4.3 NO2 total columns

Black entries relate to the setup applied to direct sun measurements, blue to direct moon.

Filters used	OPEN OPEN (no diffuser)
Effective height	BL+NO2s BL+NO2s
Number of fitting windows	2 2
Reference	Synthetic reference spectrum from solar measurements, Synthetic reference spectrum from solar measurements
Wavelength window	400.0 nm - 470.0 nm 400.0 nm - 470.0 nm
Order of polynomials	SMO 4, OFFS 0, WLC 0 SMO 4, OFFS 0, WLC 0
Fitted gases	1: H2O (BL-clim), I2 (BL-clim), NO2 (BL-clim), O2O2 (O2O2-clim), O3 (O3-clim), OIO (BL-clim) 2: H2O (BL-clim), I2 (BL-clim), NO2 (NO2s-clim), O2O2 (O2O2-clim), O3 (O3-clim), OIO (BL-clim) 1: H2O (BL-clim), I2 (BL-clim), NO2 (BL-clim), O2O2 (O2O2-clim), O3 (O3-clim), OIO (BL-clim) 2: H2O (BL-clim), I2 (BL-clim), NO2 (NO2s-clim), O2O2 (O2O2-clim), O3 (O3-clim), OIO (BL-clim)
Molecular scattering	Subtracted Subtracted

Test time series of total column NO2 at Rome-SAP showing Pandora 117 in red (sun), green (moon) and Pandora 138 in blue (sun), purple (moon). Moon data are 1h averages.

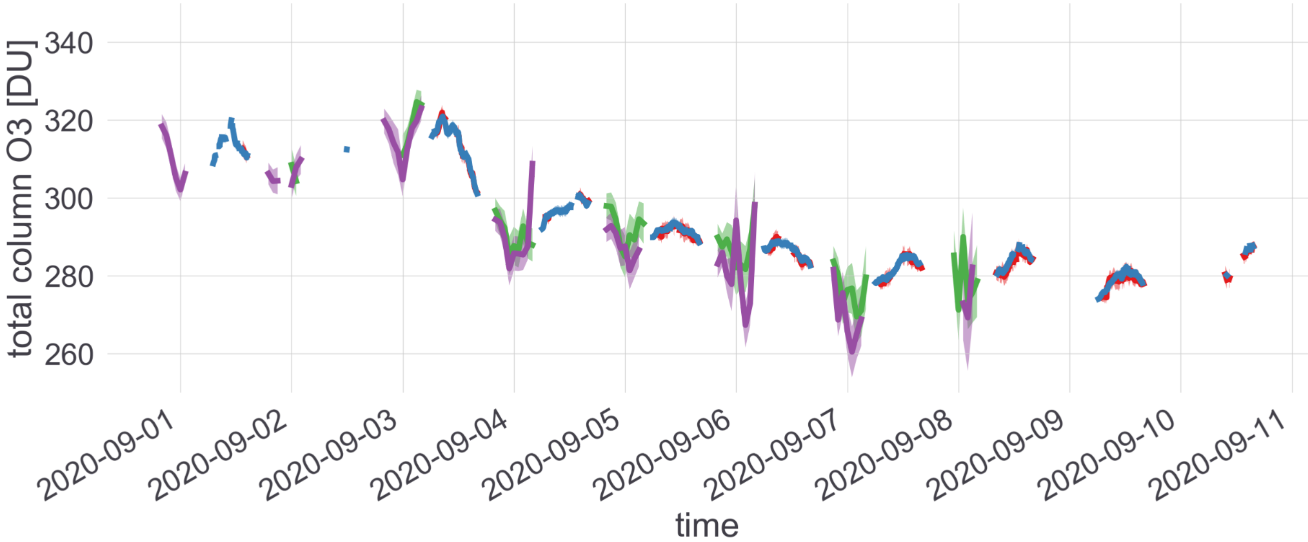


4.4 O3 total columns

Black entries relate to the setup applied to direct sun measurements, blue to direct moon.

Filters used	U340 OPEN (no diffuser)
Effective height	O3 O3
Number of fitting windows	1 1
Reference	Synthetic reference spectrum from solar measurements Synthetic reference spectrum from solar measurements
Wavelength window	305.0 nm - 333.0 nm 460.0 nm - 580.0 nm
Order of polynomials	SMO 2, OFFS 0, WLC 0 SMO 7, OFFS 0, WLC 0
Fitted gases	BrO (O3-clim), HCHO (BL-clim), HONO (BL-clim), NO2 (BL-clim), O3 (T-fit), SO2 (BL-clim) H2O (BL-clim), NO2 (BL-clim), NO3 (BL-clim), O2O2 (O2O2-clim), O3 (O3-clim)
Molecular scattering	Subtracted Subtracted

Test time series of total column O3 at Rome-SAP showing Pandora 117 in red (sun), green (moon) and Pandora 138 in blue (sun), purple (moon). Moon data are 1h averages.



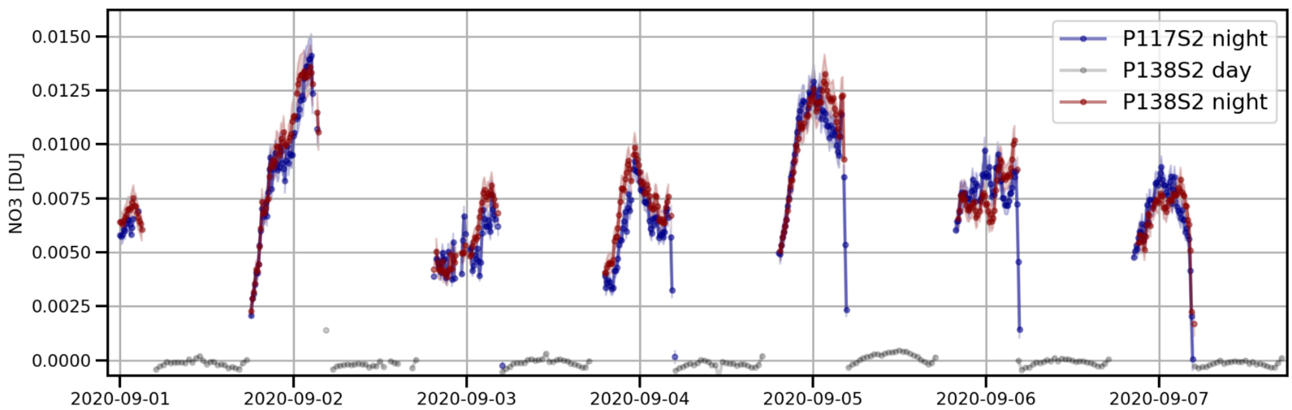
Please note that O3 retrievals in the Chappuis band have been tested the first time for Pandora. Lunar O3 column retrievals in the UV (like for sun observations) failed due to both enhanced stray light (no band pass filter could be used) and low signal zu noise.

4.5 NO3 total columns

Black entries relate to the setup applied to direct sun measurements, blue to direct moon.

Filters used	OPEN OPEN (no diffuser)
Effective height	BL BL
Number of fitting windows	1 1
Reference	Synthetic reference spectrum from solar measurements Synthetic reference spectrum from solar measurements
Wavelength window	600.0 nm - 685.0 nm 600.0 nm - 685.0 nm
Order of polynomials	SMO 4, OFFS 0, WLC 0 SMO 4, OFFS 0, WLC 0
Fitted gases	H2O (BL-clim), NO2 (BL-clim), NO3 (BL-clim), O2O2 (O2O2-clim), O2 (O2-clim), O3 (O3-clim) H2O (BL-clim), NO2 (BL-clim), NO3 (BL-clim), O2O2 (O2O2-clim), O2 (O2-clim), O3 (O3-clim)
Molecular scattering	Subtracted Subtracted

Test time series of total column NO3 at Rome-SAP showing Pandora 117 in gray (sun), blue (moon) and Pandora 138 in red (moon). Moon data are 10min averages.



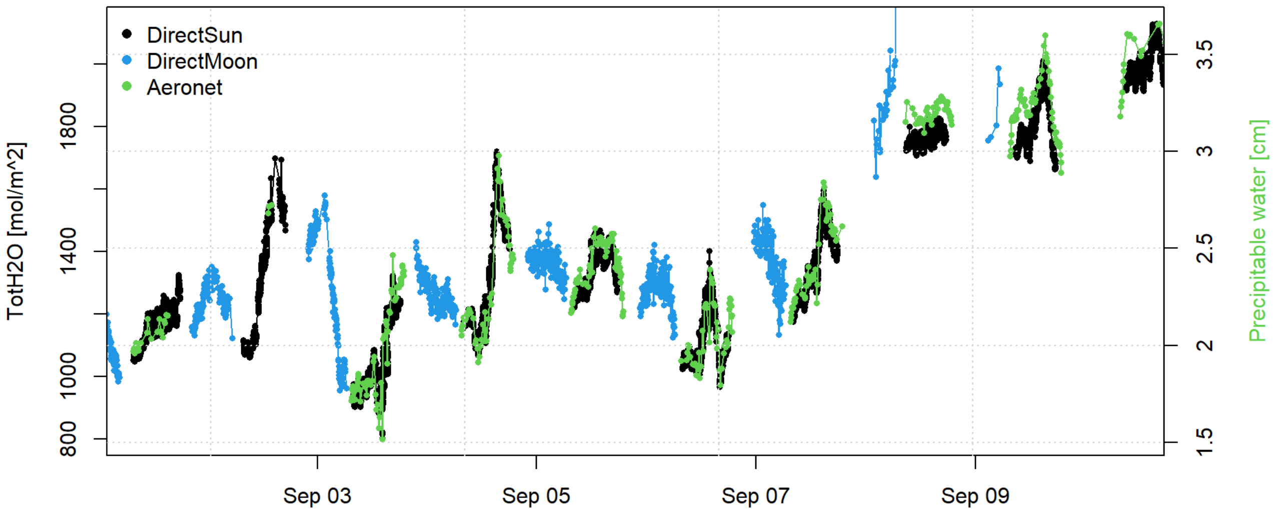
Note that next to NO3 columns from lunar observations also the column retrievals from sun observations are prototypes!

4.6 H2O total columns

Black entries relate to the setup applied to direct sun measurements, blue to direct moon.

Filters used	OPEN OPEN (no diffuser)
Effective height	BL BL
Reference	Synthetic reference spectrum from solar measurements Synthetic reference spectrum from solar measurements
Wavelength window	495.0 nm - 515.0 nm 495.0 nm - 515.0 nm
Order of polynomials	SMO 2, OFFS 0, WLC 0 SMO 2, OFFS 0, WLC 0
Fitted gases	H2O (BL-clim), NO2 (BL-clim), O3 (O3-clim) H2O (BL-clim), NO2 (BL-clim), O3 (O3-clim)
Molecular scattering	Subtracted Subtracted

Test time series of total column H2O at Rome-SAP showing Pandora 138 in black (sun), blue (moon). For comparison, the operational AERONET precipitable water product is shown in green.



Note that next to H2O columns from lunar observations also the column retrievals from sun observations are prototypes!