Fiducial Reference Measurements for Ground-Based DOAS Air-Quality Observations

ESA Contract No. 4000118181/16/I-EF - CCN03

Deliverable D26:

NDACC MAX-DOAS Service Performance Assessment Report

Date: 15/04/2021

Version: 2.0

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We would like to thank Roger Lin (NOAA) and Ann Mari Fjaeraa (NILU) for their support in establishing the data flow between the FRM$_4$DOAS database and the NDACC and EVDC data handling facilities.

Content

1 Introduction

This report is an update of the first version of the deliverable D26 'NDACC MAX-DOAS Service performance assessment report' submitted to ESA on 14 December 2020. The new document (version 2.0) reflects the status of the service at the end of CCN03 (i.e. as on 31 March 2021) and is structured as follows: the assessment of the Central Processing System (CPS) performance in terms of computing time and input/output data storage size carried out during CCN02 is provided as reminder in Sect. 2. A description of the data stream between the FRM_4DOAS database and the NDACC and EVDC data handling facilities (DHFs) is given in Sect. 3. The current status of the submission of the FRM_4DOAS GEOMS files to the NDACC and EVDC DHFs and the status of the NDACC affiliation procedures for partners' instruments are presented in Sect. 4 and 5, respectively. As conclusion, the main lessons learned about the Service during CCN03 are discussed in Sect. 6.

2 CPS performance assessment

The assessment of the CPS in terms of computing time and input/output data files storage size is presented here. Both parameters are evaluated based on the central processing of one day (20/06/2020) of level-1 spectra files for two different instruments: the Bremen UV and VIS dual-channel and the Athens UVVIS single channel instruments (~55 and ~330 MAX-DOAS scans per day for the selected day, respectively). Results are presented in Table 1 and Table 2, respectively. This evaluation, which was presented in the CCN02 deliverable D21, is still valid since the same version of the processor is currently used in the NDACC MAX-DOAS Service.

	L1	QDOAS/ QDOAS_QAQC	TROPO ~55 scans (~330 scans)	NO2strato	O3total	TOTAL
Channel 1 - UV	15s	30s	12 min	-	-	~13 min
Channel 2 - VIS	15s	30s	10 min	~15s	~15s	~11 min
Athens	15s	30s	70 min	~15s	~15s	70 min

Table 1. Computing times corresponding to the different steps of the central processing.

	L1 (MB)	QDOAS /_QAQC (MB)	TROPO (MB)	NO2strato (MB)	O3total (MB)	TOTAL (MB)
Channel 1 - UV	~3 (x2)	~1 (x2)	~4	-	-	~12
Channel 2 - VIS	~3 (x2)	~1 (x4)	~3	~0.3	~0.3	~14
Athens	~15 (x2)	~3 (x4)	~15	~0.3	~0.3	~60

Table 2. Storage sizes corresponding to the different intermediate products of the central processing. For level-2 products, the storage sizes correspond to the sum of the sizes of the GEOMS and netCDF master files. However, those sizes are largely dominated by the netCDF master files, the GEOMS file ranging only between a few tens of kB for stratospheric products to a few hundreds of kB for tropospheric products.

As can be seen from Table 1, the computing time is the largest for the TROPO retrieval step (~12 min per channel for the Bremen instrument and 70 min for the Athens spectrometer, in comparison to ~15s for total O_3 column

and stratospheric NO_2 profile retrievals). Given the fact that there are less measurement scans in winter than in summer, input/output files represent a total 10-20 GB per year per instrument. It should be noted that only the TROPO and total O_3 products are currently delivered (GEOMS format) as part of the NDACC MAX-DOAS Service.

3 FRM$_4$DOAS data stream to NDACC and EVDC

The submission of the level-2 GEOMS HDF4 files from the FRM4DOAS database to the NDACC data handling facility is controlled by a dedicated wrapper which makes use of trigger lists (see FRM$_4$DOAS CCN02 deliverable D20 'MAXDOAS_Network Operational Processing System Architecture Design Document'). Based on the instrument configuration files, profiling wrappers generate trigger lists with the names of the GEOMS files that are produced by the Central Processing System. The NDACC wrapper is executed once per day (at 15:30 UTC) and submits the files included in the trigger lists, corresponding to the day before to the NDACC incoming ftp site ftp.hq.ncep.noaa.gov/pub/incoming/ndacc at NOAA. Those files then pass the NDACC QA/QC checks before their cataloging on the NDACC rapid delivery (RD) repository (ftp://ftp.cpc.ncep.noaa.gov/ndacc/RD/). The submission to EVDC is done via a mirroring approach (consistency checks between NDACC and EVDC databases and transfer of the new NDACC files that are not present on the EVDC database to the latter).

A description of this data stream is presented in Figure 1.

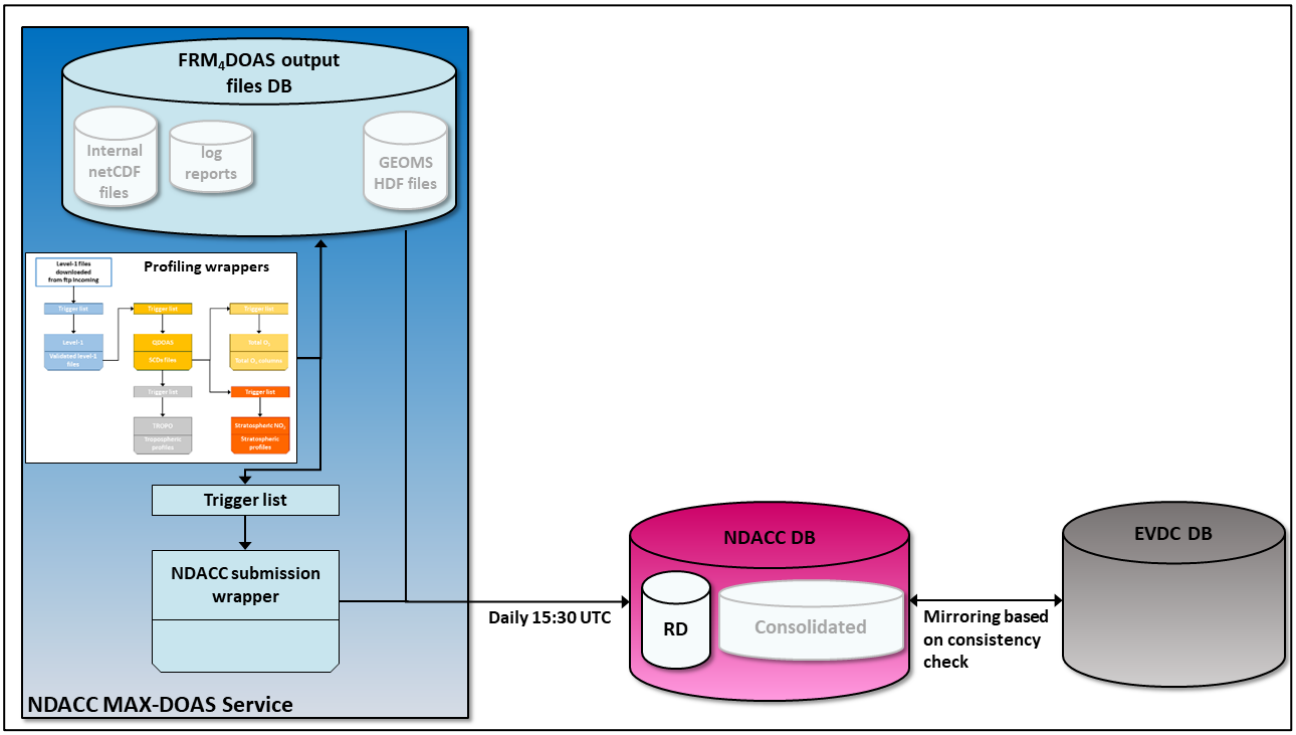

Figure 1. FRM$_4$DOAS data stream to NDACC and EVDC. Only the MAX-DOAS tropospheric NO_2 and twilight zenith-sky total O_3 products are currently submitted on NDACC and EVDC (see Sect. 4).

4 FRM$_4$DOAS data submission to NDACC and EVDC: current status

The status of the FRM4DOAS GEOMS HDF4 files submission to the NDACC and EVDC DHFs is presented in Table 3. It should be noted that only the MAX-DOAS tropospheric NO_2 and twilight zenith-sky total O_3 products have been assessed to be mature enough for their public release on NDACC and EVDC.

Instr #	Station name	affiliation	Geometry	Level-1 daily sub. status	TOTAL O3	TROPO NO2	Level-2 sub. to NDACC RD (+ mirroring on EVDC)
1669	XIANGHE	BIRA.IASB	Maxdoas	X	X	X	Daily since 10/2020
1671	HARESTUA	BIRA.IASB	Zenith	X	X	N/A	Daily since 10/2020
1672	NY.ALESUND	IUP	Maxdoas	X	X	X	Daily since 02/2021
1673	BREMEN	IUP	Maxdoas	X	X	X	Daily since 12/2020
1674	ATHENS	IUP	Maxdoas	X	X	X	Daily since 12/2020
1676	MAINZ (x4)	MPIC	Maxdoas	X	N/A	X	Daily since 12/2020
1677	LAUDER	NIWA	Maxdoas	w	X	X	Bi-weekly since 01/2021
1678	NEUMAYER	UHEIDELBERG	Maxdoas	X	X	X	Daily since 01/2021
1679	HEIDELBERG	UHEIDELBERG	Maxdoas	X	X	X	Daily since 12/2020
1683	THESSALONIKI_AUTH	AUTH	Maxdoas	X	N/A	X	Daily since 12/2020
1684	DEBILT	KNMI	Maxdoas	X	N/A	X	Daily since 03/2020
1686	THESSALONIKI_AUTH	AUTH	Maxdoas	X	X	X	Daily since 12/2020
1698	IZANA	INTA	Maxdoas	w	X	MTS	Bi-weekly since 12/2020
1670	UCCLE	BIRA.IASB	Maxdoas	-	X	X	07/2018-02/2020
1675	DEBILT	KNMI	Maxdoas	-	X	X	07/2018-11/2019
1684	LA.REUNION.MAIDO	BIRA-IASB	Maxdoas	-	X	MTS	07/2018-12/2019
1688	DEBILT	KNMI	Maxdoas	-	N/A	X	12/2020-01/2021
1682	UTSTEINEN	BIRA.IASB	Maxdoas	Central processing under testing			
1689	UCCLE	BIRA.IASB	Pandora	Central processing under testing			

Table 3. Status of FRM$_4$DOAS GEOMS HDF data files submission to NDACC and EVDC. 'w' stands for ~weekly submission of level-1 spectra files to the CPS, 'N/A' for algorithm not applicable, and 'MTS' for mountain-top station (only total O_3 files submitted to NDACC). Due to the low tropospheric NO_2 content (+instrumental issue in the case of Ny-Alesund; see Sect. 6), the retrieval of tropospheric NO_2 at Ny-Alesund and Neumayer is still under testing (-> orange instead of green crosses in the Table).

The daily automatic file submission started beginning of December 2020 for most of the stations. The stations of the different partners can be classified as follows in term of file submission frequency to NDACC and EVDC DHFs (see Table 3):

- Daily automatic submission: Xianghe, Harestua, Ny-Alesund (total O_3 only), Bremen, Athens, De Bilt (3 different instruments were used to ensure a complete data set since July 2018, see Figure 3), Mainz, Neumayer (total O_3 only), Heidelberg, Thessaloniki (instruments 1683 and 1686)
- ~Bi-weekly automatic submission: Lauder, Izaña
- NRT central processing and automatic data stream to NDACC and EVDC stopped: Maïdo (instrumental issue), Uccle (instrument temporarily dismantled; replacement by a Pandora system under progress), De Bilt (submission of spectra from 1675 and 1688 instruments stopped; only 1684 in use for the NDACC MAX-DOAS Service)
- Central processing under testing for Utsteinen (Max-DOAS) and Uccle (Pandora)

It should be noted that the files currently catalogued successfully passed the NDACC QA/QC checker but are also compliant with the CAMS-27 QA/QC criteria, even if - because of the demonstration mode - they are not ingested in CAMS-27 for the moment.

When available, past measurements from July 2018 (official start of the central processing system) to December 2020 have been reprocessed by the CPS and corresponding GEOMS files submitted to the NDACC RD repository (with mirroring on EVDC) in January 2021. The temporal coverages of both total O_3 and tropospheric NO_2 products at the partners' stations are presented in Figures 2 and 3, respectively.

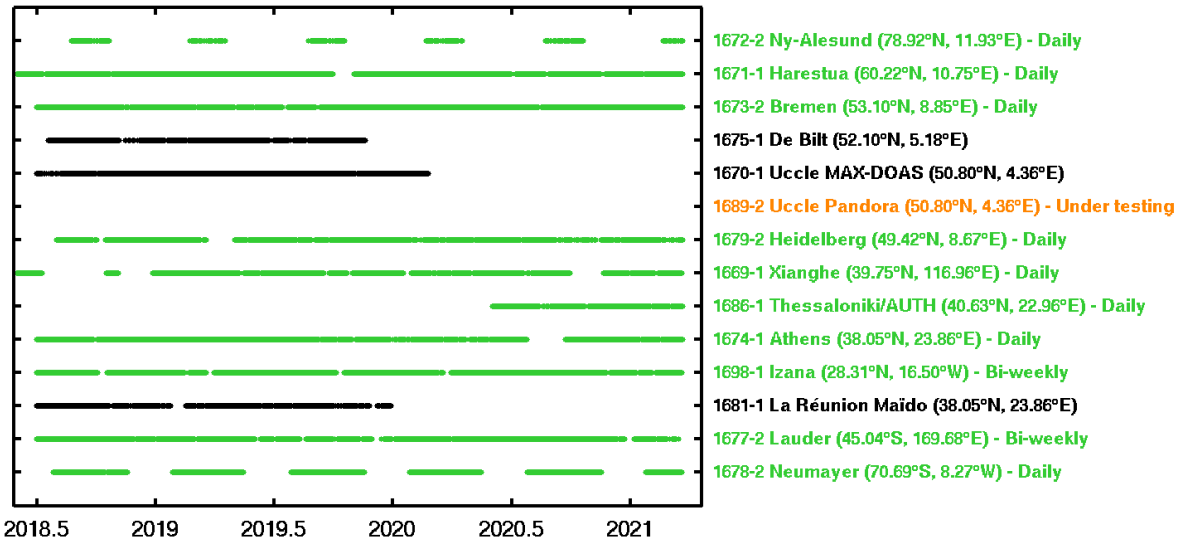

Figure 2. Temporal coverage of the NDACC MAX-DOAS Service total O_3 product on the NDACC/RD and EVDC DHFs as on end of March 2021. Time-series for instruments in operation, stopped, and under testing appear in green, black, and orange, respectively.

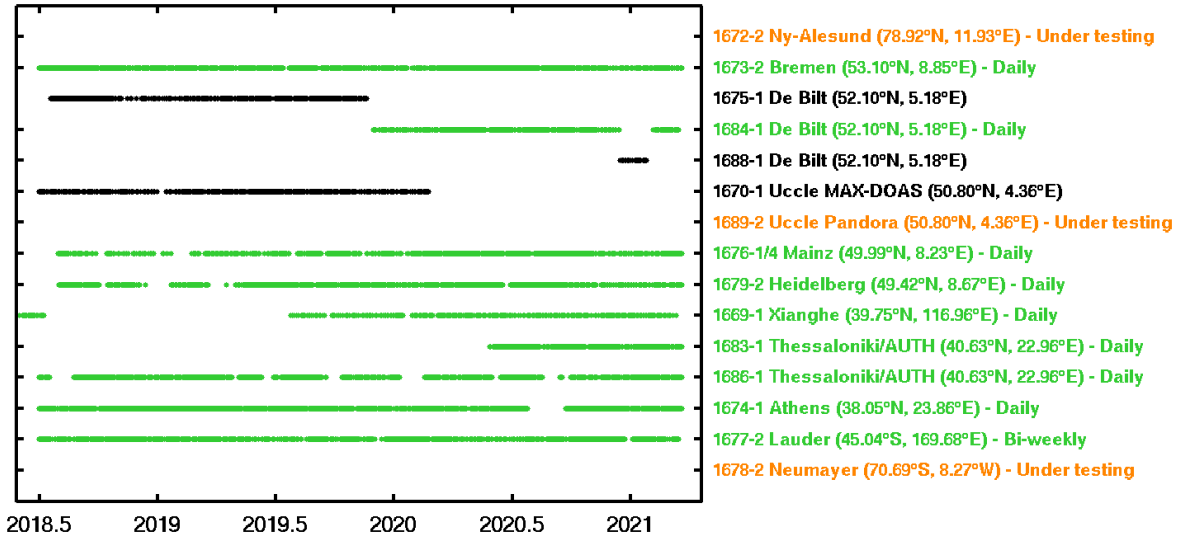

Figure 3. Temporal coverage of the NDACC MAX-DOAS Service total NO_2 product on the NDACC/RD and EVDC DHFs as on end of March 2021. Time-series for instruments in operation, stopped, and under testing appear in green, black, and orange, respectively. It should be noted that in the case of De Bilt, 3 different instruments were used to ensure a complete data set since July 2018.

5 NDACC affiliation procedure

Progressing in the NDACC affiliation procedure for the partners' stations was one of the task of this CCN03. Table 4 presents the status of the affiliation procedure at the beginning of CCN03. The current status can be summarized as follows:

- Bremen, Athens: Minimal input needed from IUP-Bremen, then the NDACC UV-vis co-chairs can proceed with the affiliation letters.
- De Bilt: KNMI has informed the NDACC UV-vis co-chairs about their wishes in terms of the NDACC affiliation of their MAX-DOAS instruments.

- Lauder (NIWA101 instrument): Letter of affiliation request has been updated for also including Macquarie Island (NIWA102 instrument) and Arrival Heights (NIWA103 instrument) in addition to Lauder and has been sent to the NDACC co-chairs.
- Arrival Height (ADAS2 instrument jointly operated by UHEID and NIWA, with UHEID as PI): Letter of affiliation request sent to the NDACC co-chairs.
- Heidelberg: UHEID has provided the necessary information for affiliation to the NDACC UV-vis co-chairs.
- Thessaloniki: All the necessary information have been received for the new instrument and the NDACC UV-vis co-chairs will now proceed with the affiliation letter.
- Uccle (Pandora instrument) and Reunion/Maïdo (MAX-DOAS instrument): the affiliation of those instruments is postponed. In the case of Uccle, a few more months is needed for optimization of the Pandora acquisition sequence and verification of the corresponding FRM$_4$DOAS retrieval settings and results. Regarding Reunion, a re-localisation of the instrument from the Maïdo observatory to the coastal region is under discussion.

The above affiliation procedures will continue after CCN03.

Site	NDACC affiliation status	To be affiliated (Y/N)	Instrument(s)	Institute	Instrument PI
Xianghe	NA	N	MAX-DOAS	BIRA-IASB/IAP	Michel Van Roozendael/Pucai Wang
Uccle La Reunion	NA NA	Y Y	Pandora MAX-DOAS	BIRA-IASB	Michel Van Roozendael
Harestua	A	--	ZSL-DOAS	BIRA-IASB	Van Roozendael
Ny-Alesund	A	--	MAX-DOAS	IUP-Bremen	Andreas Richter
Izana	A	--	MAX-DOAS	INTA	Monica Navarro
Bremen Athens	NA NA	Y Y	MAX-DOAS MAX-DOAS	IUP-Bremen	Andreas Richter
De Bilt	NA	Y	EnviMes	KNMI	Ankie Piters
Mainz	NA	N	Tube-DOAS	MPIC-Mainz	Thomas Wagner
Lauder	NA	Y	EnviMes	NIWA	Richard Querel
Neumayer	A	--	MAX-DOAS	U. Heidelberg	Udo Friess
Heidelberg Arrival Height	NA NA	Y Y	MAX-DOAS MAX-DOAS	U. Heidelberg	Udo Friess
Thessaloniki	NA	Y	Phaeton	AUTH	Alkis Bais

Table 4. Status of the NDACC affiliation procedure of FRM4DOAS' partners instruments at the beginning of CCN03. The color code is: **green (to be affiliated)**, **blue (already affiliated)**, **orange (no affiliation planned in the short term)**.

6 Main lessons learned during FRM$_4$DOAS CCN03

As conclusion, the main lessons learned during FRM$_4$DOAS CCN03 and which are important in the perspective of the future operational system are discussed here and more details can be found in the final presentation of CCN03 available on the FRM$_4$DOAS ftp server ftp-ae.oma.be, in /FRM4DOAS_project/Meetings/CCN03_FM_Telecon_20210325/Presentations. Those lessons are:

1. Need for continuous monitoring of the DOAS fit RMS and errors as part of the routine QA/QC checks: During CCN03, those parameters were examined off-line for the different instruments, and in the case of Ny-Alesund, a degradation (increase) of both parameters with time was found, from October 2018 (see Figure 4) leading to a significant reduction of the DOFS for the tropospheric and stratospheric NO_2 profile retrievals. This degradation was related to an instrumental issue (problem with the quartz fiber bundle which reduced light throughput by nearly one order of magnitude).

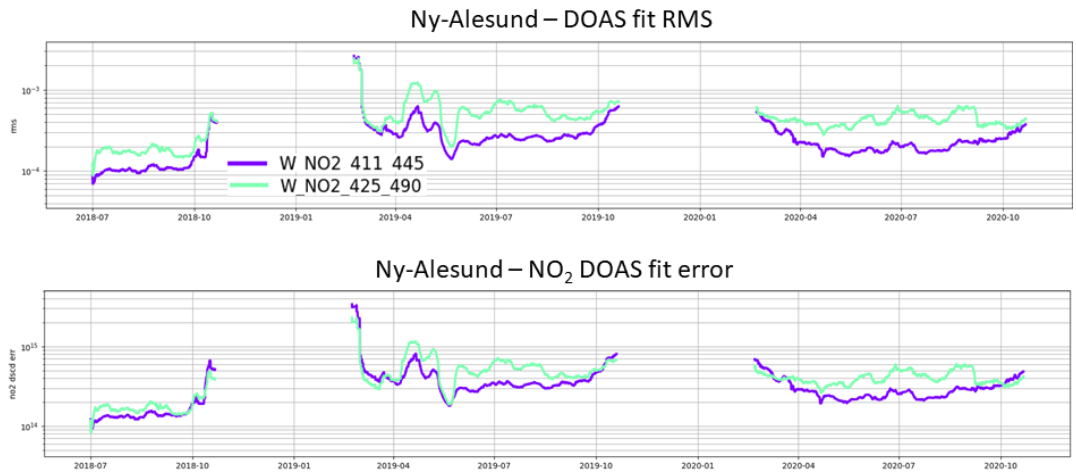

Figure 4. Evolution of the DOAS fit RMS and NO_2 DOAS fit error (411-445nm and 425-490nm fitting windows) for the Ny-Ålesund instrument since July 2018. Both curves correspond to rolling 10-day medians.

2. Need for further refinements of the QA/QC flagging approach for the tropospheric NO_2 product: The impacts of the QC flags currently implemented in the tropospheric QA/QC flagging approach, i.e. the consistency flag (at least MMF or MAPA code should be valid + MMF and MAPA VCD within their combined errors) and the extra DSCD error flag (scans with large difference between the zenith DSCD before and after the scan compared to the DOAS fit error are flagged as invalid), were examined at different stations. For high S/N ratio research-grade instruments like in Athens, the extra DSCD error flag is found to reduce the number of valid scans and also to produce less marked NO_2 peaks, creating a bias toward clean situations (see Figure 4). For the other types of instrument (like in De Bilt), the extra DSCD error has a limited impact on the retrieval results. These findings appeal for further investigations on the extra DSCD error flag and its effect on the tropospheric NO_2 retrievals. A first test to be done is to relax the factor of 3 which is currently used as upper limit for the difference between the extra DSCD error and the DOAS fit error.

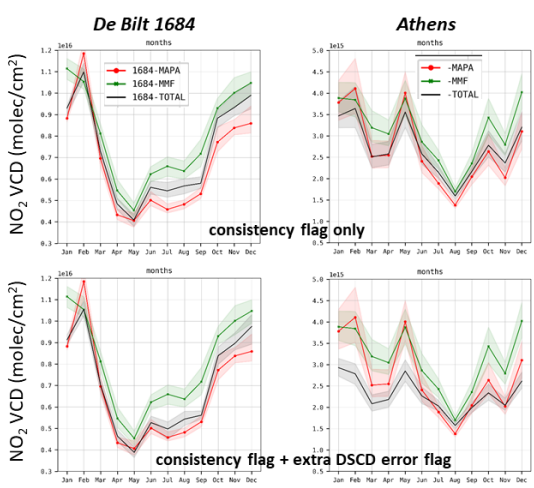

Figure 5. Seasonal variation of the NO_2 VCD (monthly medians) at the De Bilt (left) and Athens (right) stations. Green and red curves correspond to the MMF and MAPA results (monthly medians and 45% and 55% percentiles), respectively. Black curves correspond to the MMF results after applying the consistency flag only (upper plots) and the consistency and extra DSCD error flags (lower plots).

3. Need for a thorough characterization of the measurement site by the PIs before submitting first spectra files to the CPS: The examination of the retrieved tropospheric NO_2 vertical profiles in the UV, VIS, and UVVIS channels at Lauder indicated that the retrieval results could be potentially impacted by a mountain area located at ~42km from the station (see Figure 6). An elevation scan done by NIWA in the pointing direction of the instrument showed that the mountain area was indeed an obstacle for the 1° elevation measurements. For entering into the future operational processing system, PIs should perform an assessment of their measurement site(s) through a dedicated questionnaire (to be created). If potential obstacle(s) are present in the pointing direction(s), it should be the role of the PIs to inform the CPS operators and to further characterize the measurement environment through additional tests like elevation scan(s). Making the list of available ancillary observations at the measurement site could be also useful for an eventual validation/verification of the retrieval results generated by the CPS.

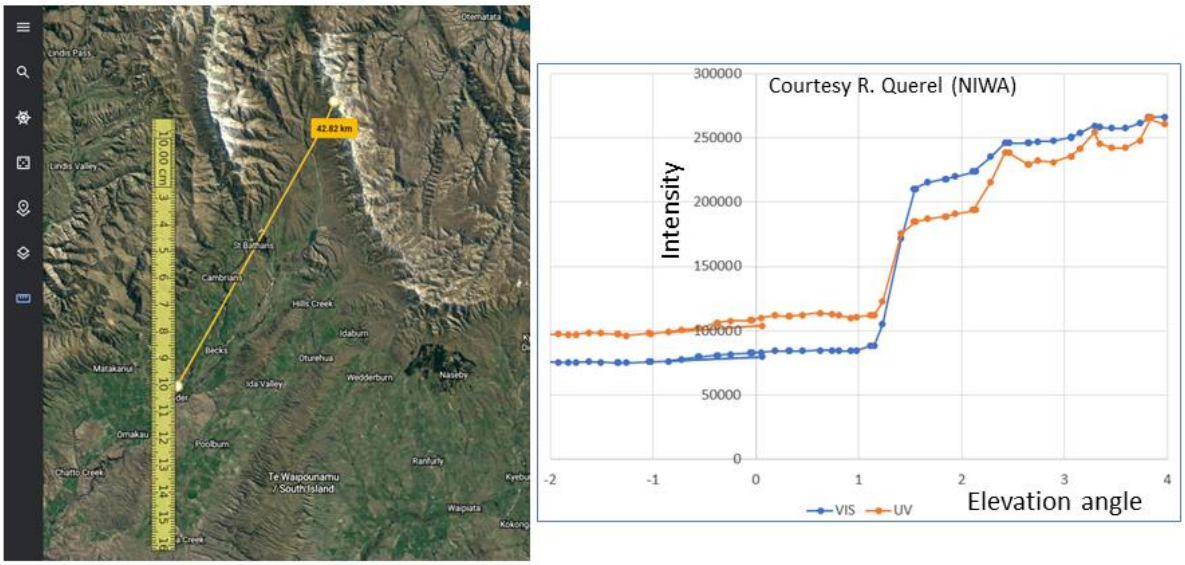

Figure 6. Google map showing the environment around the Lauder station (left) and results of the horizon scan (right).

4. Need for a PI-web-interface, where PI can submit preferred alert-notification settings and necessary station information, and where PI can view instrument and processing status.