



D-1 Report on TROPOGAS compliance/difference with FRM4DOAS requirements

'WPs 2250-2251: DOAS-BO: Towards a new FRM4DOAS-compliant site'

Document reference:	FRM4DOAS-BO_D1
Document Issue:	1.0
Document Issue date:	04/03/2021
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TABLE OF CONTENTS

1	LIST OF ACRONYMS	2		
2	INTRODUCTION	2		
3	PROJECT TASKS	2		
	3.1 WP2250-1.1: QUALITY REQUIREMENTS, REVIEW OF LITERATURE AND COMMUNICATION	TION WITH FRM4DOAS		
	COMMUNITY	2		
	3.2 WP2250-1.2: ASSESSMENT OF TROPOGAS PERFORMANCES	3		
	3.2.1 The TROPOGAS UV-Vis system	3		
	3.2.2 TROPOGAS performance assessment vs FRM4DOAS requirements	5		
	3.2.3 Example of TROPOGAS netCDF Level-1 file	10		
4	CONCLUSIONS	12		
5	REFERENCES 13			

AMENDMENT RECORD SHEET

The Amendment Record Sheet below records the history and issue status of this document.

ISSUE	DATE	REASON
1.0	04/03/2021	D-1 document of project "WPs-2250-2251: DOAS-BO: Towards a new FRM4DOAS-compliant site'".





1 List of Acronyms

CCD	Charge-Coupled Device
DAS	Data Acquisition System
DOAS	Differential Optical Absorption Spectroscopy
ERF	Error Function
EU	Electronic Unit
FOV	Field Of View
FWHM	Full Width Half Maximum
FRM4DOAS	Fiducial Reference Measurements for DOAS
GASCOD	Gas Analyser Spectrometer Correlating Optical Differences
GAW	Global Atmospheric Watch
ISAC	Istituto di Scienze dell'Atmosfera e del Clima
LOS	Line of Sight
MAX-DOAS	Multi AXis – DOAS
NDACC	Network for the Detection of Atmospheric Composition Change
OU	Optical Unit
SCD	Slant Column Densities
SNR	Signal to Noise Ratio
SODCAL	Scanning Optical Device Collecting Atmospheric Light
TROPOGAS	Tropospheric Gas Analyzer Spectrometer
UV-Vis	UltraViolet-Visible
WMO	World Meteorological Organization

2 Introduction

This document is the report of the activities performed in the frame of the two first WPs (1.1 and 1.2) of the "WPs-2250-2251: DOAS-BO: Towards a new FRM4DOAS-compliant site" project.

3 Project tasks

The WPs 1.1 and 1.2 of the project are mainly centred on the review of the available literature on best practices for DOAS and MAX-DOAS stations and data processing and the assessment of the TROPOGAS performances, compliances and not with respect to requirements identified by the FRM4DOAS network.

3.1 WP2250-1.1: Quality requirements, review of literature and communication with FRM4DOAS community

The FRM4DOAS project is an ESA project that aims at harmonization of MAX-DOAS systems and data sets, through the

• specification of best practices for instrument operation





- demonstration of a centralised NRT (near-real-time/6-24h latency) processing system for MAXDOAS instruments operated within the international NDACC
- establishment of links with other UV-Visible instrument networks, e.g. Pandonia.

(bullets from https://frm4doas.aeronomie.be)

In the frame of the WP 1.1, we focused on the analysis of the best practices suggested by FRM4DOAS to be applied to the TROPOGAS instrument for both the measurements set-up and the Level-1 file format.

The two reference documents used for this study are: FRM4DOAS Instrument Operation and Calibration Guidelines [R1] and FRM4DOAS Level-1 data [R2].

In [R3], an extended version of [R1], we can find instrumental, operational and data processing guidelines.

For each of these requirements, we analysed the TROPOGAS compliances or not and identified the operational and processing changes that we will apply to our measurement and data analysis strategy. A detailed description of this process is given in section 3.2.2.

The Level-1 output of MAX-DOAS systems part of the FRM4DOAS network are netCDF files containing the spectra measured by the instrument together with several ancillary but fundamentals information such as viewing angles (azimuth and elevation), latitude and longitude, wavelength grid and so on. The netCDF format described in [R2] is suitable for the centralized NRT processing described above.

An example of TROPOGAS spectra in netCDF FRM4DOAS compliant format is given in the section 3.3.3.

Nevertheless, FRM4DOAS netCDF data format can be used by the QDOAS (http://uvvis.aeronomie.be/software/QDOAS/) algorithm to process DOAS and MAX-DOAS spectra in order to obtain SCDs of species with spectral features in UV and Vis spectral ranges (QDOAS version 3.4 -11 March 2020). Thus, in the frame of this project, we will use the QDOAS software package to process TROPOGAS spectra.

In order to choose the best retrieval configurations for our analysis, we had some email interactions with the QDOAS team.

3.2 WP2250-1.2: Assessment of TROPOGAS performances

Before assessing the performances of the TROPOGAS instrument, we give an overview of the instrument itself, of its heritage and its geographical position in Northern Italy at the edge of the Po Valley. Then, we will assess its performances with respect to the FRM4DOAS requirements as specified in [R1] and [R3]. We will also give an example of the TROPOGAS netCDF Level-1 file.

3.2.1 The TROPOGAS UV-Vis system

The TROPOGAS is a remote sensing UV-Vis system for DOAS applications. The system belongs to the family of the GASCOD spectrometers [R4] developed at ISAC-CNR. The first GASCOD spectrometers were installed in the GAW-WMO Mt. Cimone station in 1993 for zenith sky measurements, and in the Mario Zucchelli station in Terranova





Bay in 1995. In recent years (2016), a MAX-DOAS system has been installed in the Lecce Atmospheric observatory. Companion systems, the SPATRAMs, are installed in Evora [R5].

The TROPOGAS spectrometer has a spectral resolution of about 0.4 nm in the UV region and of 0.5 nm in the visible and measures zenith and off-axis atmospheric scattered radiation in the spectral region from 300 to 600 nm.

In the core of the spectrometer the radiation is measured by a CCD sensor of 1054 x 254 pixels (each one of 0.025 mm wide resulting in a sampling step of 0.06nm). Of those pixels 1024 x 254 are illuminated and the remaining are used as dark reference. For spectral analysis, the 254 columns are binned in groups of 41 to improve the signal to noise ratio as well as the time resolution of the measurements. The sensor is cooled at -35°C to reduce the CCD thermal noise and dark current.

The TROPOGAS spectrometer is coupled with an Alt azimuth platform, developed and implemented at ISAC and called SODCAL, by means of an optical fibre and it is used for off-axis and zenith sky measurements of diffuse solar radiation. The Alt Azimuth Platform is a small telescope with a mirror objective with a diameter of 60 mm resulting in a FOV of few degrees, and both azimuth and zenith movements that transmits the radiation collected at a given LOS to the spectrometer by means of an optical fibre. The cycle of pre-defined measurements is composed by a set of off-axis and zenith sky measurements.

More details on the system can be found in [R5] and [R6].



Figure 1: TROPOGAS instrument with Alt Azimuth platform on the CNR-ISAC roof in Bologna.

The TROPOGAS spectrometer is placed on the roof of the ISAC-CNR institute in Bologna (in the OpenLab 44.523669° N, 11.338346° E, 54 m a.s.l.), a few kilometres outside the city centre in the North (urban background) since 2018. The system has





also been used in measurement campaigns to study cruise ship flow rate emissions in Venice lagoon area [R6] and chimney emissions.

3.2.2 TROPOGAS performance assessment vs FRM4DOAS requirements

As reported in section 3.1, FRM4DOAS network provides instrumental, operational and data processing guidelines that DOAS measurements should meet. These guidelines are divided into three groups: instrumental, operational and data processing guidelines. The details of the guidelines and the compliance of the TROPOGAS instrument with respect to them is reported in the following.

3.2.2.1 Instrumental guidelines

At least one O4 band covered well TROPOGAS meets this requirement completely, indeed i

TROPOGAS meets this requirement completely, indeed it measures the diffuse solar radiation in several spectral bands from 300 to 600 nm, covering well different O4 bands, in particular the one located at about 475 nm.

- Quartz fiber for removal of polarization features The Alt azimuth platform (SODCAL) is connected to the TROPOGAS spectrometer, located indoor, by means of a quartz fiber.
- Optical low pass filter for straylight removal in UV
 Straylight bias can affect the acquired spectra, mainly in the UV region and it consists of undesired visible light reaching the CCD sensor. To avoid it, the TROPOGAS has an optical low pass filter that can be used during UV measurements.

• Proper time information

Every acquired spectrum is coupled with the proper time information by the acquisition software.

• Spectral resolution better than 0.8 nm (UV) and 1.5 (visible)

For the spectral resolution estimate, the QDOAS software has been exploited. During the QDOAS spectral calibration procedure, spectra are compared to the high resolution tabulated solar spectrum [R8]. The tabulated solar spectrum is iteratively degraded (by the convolution with different gaussian slit functions) until the best match with the measured spectrum is reached (for further information see [R9]). The slit function FWHM represents an estimate of the spectral resolution. Figure 2 shows that TROPOGAS completely meets the requirement, since it has a quite constant high spectral resolution of about 0.35 nm.







Figure 2: temporal evolution of the TROPOGAS spectral resolution.

• FOV better than 1.5° in vertical direction

The field of view has been estimated exploiting the horizon scan method, explained in [R7]. We have measured the signals at 440 nm for different elevation angles around the horizon. We have chosen a clear day in order to be able to observe a contrast between earth and sky.

The blue dots in figure 3 show that the signal at 440 nm is near 0 for low elevation angles (when the whole detected signal comes from the earth). Increasing the elevation angle, part of the FOV starts to detect the sky and the signal increases until the elevation angle is big enough and all the signal reaching the FOV comes from the sky.

The blue dots are fitted by the function S (blue line):

$$S = A \left[ERF\left(\frac{x - x0}{B}\right) + 1 \right] + C$$

where ERF is the error function and A, B, C and x0 are fitted parameters. The red curve is a Gaussian and represents the derivative of the S analytical function. Its FWHM is a FOV estimate and is computed as:

$$FWHM = 2\sqrt{\ln(2)}B$$

The estimated TROPOGAS FOV is 3.6°, as reported in the figure 3 title. Since the FOV required by FRM4DOAS standard is 1.5°, TROPOGAS does not meet this requirement. We plan to evaluate the impact of FOV amplitude on the MAX-DOAS measurements through radiative transfer simulations. Mitigation strategies, if possible, will be investigated. The FOV amplitude is the only instrumental requirement that is not compliant to FRM4DOAS.







DOAS-BC

Figure 3: the blue dots represent the signals measured at 440 nm for different elevation angles in an arbitrary unit. The blue line is the error function (ERF) used to fit the data. The red line is a Gaussian and is the derivative of the blue line. Its FWHM represents the FOV, as reported in the figure title.

3.2.2.2 Operational guidelines

Operational requirements have the purpose to fix a standard acquisition strategy in order to maximize the information contained in both MAX-DOAS and Zenith measurements. In particular, most of them are easily satisfied changing some files that drive the automatic data acquisition system (DAS) [R10]. These requirements are:

- SZA range up to 85° for MAX-DOAS and up to 94° for zenith-sky observations
- Zenith-sky observations at least every 30 minutes during MAX-DOAS observations
- At least one zenith-sky measurement per degree SZA at twilight
- At least 1°, 2°, 3°, 5°, 10°, 30° elevations in scan
- Horizon scan on a regular basis

The method used to estimate the FOV, described in the instrument guidelines, can also be exploited to evaluate the pointing stability, indeed the center of the Gaussian curve, in figure 3, represents the horizon elevation angle, according to TROPOGAS.

If the true horizon elevation angle is known, this strategy provides a simple pointing calibration method.

According to FRM4DOAS standards, the dark current must also be subtracted from the acquired spectra. The requirement is:

- Dark signal must be measured at least daily
 - This point has been more complicated because it required to modify the DAS code. In the previous acquisition configuration, TROPOGAS measured the dark signal together with the spectrum using additional pixels of the CCD sensor that are not used for spectra acquisition. However, figure 4 shows that the dark signal, measured in the same 1024 pixels used for atmospheric acquisitions, is dependent on the pixel. For this reason, the code has been modified in order to measure the dark signal in the same CCD pixels used to measure the atmospheric spectra.







Figure 4: Dark spectrum acquired in the same pixels used for atmospheric measurements, with an exposure time of 30 seconds and a CCD temperature of -20.2 °C.

According to this new configuration, TROPOGAS measures a dark spectrum after every atmospheric acquisition, maintaining the same measurement exposure time.

We perform dark current measurements by changing the light input of the spectrometer from SODCAL, used for solar diffuse spectra acquisition, to the calibration lamps entrance with lamps turned off.

The last required operational guideline is:

- The slit function must be measured on a regular basis (daily if possible)
 - As shown in figure 2, the spectral resolution is continuously monitored, by comparing each measured spectrum to the high resolution tabulated solar spectrum. In this way, the slit function is monitored since its FWHM represents the spectral resolution.

Thus, all the FRM4DOAS operational guidelines are met.

3.2.2.3 Data processing guidelines

• Apply dark signal correction

This operation is performed automatically during the spectra acquisition. The dark signal is measured, as explained in the operational guidelines, and subtracted to the atmospheric spectrum.

• Apply wavelength calibration

An appropriate wavelength grid is found comparing the measured spectra with the high resolution tabulated solar spectrum. For this operation, the calibration routine within the QDOAS software is exploited.

• Apply non-linearity correction

The sensor linearity has been evaluated exploiting the quartz-iodine lamp mounted inside the instrument, usually used for radiometric calibrations since it produces smooth spectra. For this test, we measured 41 quartz-iodine spectra in the spectral window centered at 333.7 nm with different exposure times from 0.2 s to 8.2 s. We have chosen this spectral window because the quartz-iodine signal is spectrally constant. Figure 5 (left) shows the signal





behavior (black dots) with respect to the exposure time for only one CCD pixel, which corresponds to one point of the spectrum. The behavior is linear everywhere except for low counts, where data are slightly higher than the linear trend.

The same method is applied to all the 1024 CCD pixels.

In the figure 5 (right), the ratios between the linear curves and data are plotted with respect to the spectra values (counts), for all the 1024 CCD pixels. All the 1024 CCD pixels are characterized by the same behavior; measurements are linear in the range between 20000 and 60000 counts, while for counts lower than 20000, data start to deviate from linearity and so they require to be corrected. Over 60000 counts, the sensor saturates. However, such high counts are never reached during automatic measurements because, before every spectrum measurement, the acquisition system automatically computes an optimal exposure time in order to have high signals without reaching the saturation.



Figure 5: In the left, counts of a single point of the spectrum (equivalent to one CCD pixel) in black with respect to the exposure time. The red line represents the perfect linear behavior. In the right, ratios between linearity (points in the red line) and data (black dots) for all 1024 CCD pixels.

• Average spectra to reach SNR of at least 3000 (visible) or 4000 (UV)

The SNR of a single TROPOGAS spectrum cannot meet the FRM4DOAS requirements. In that case, averaging different spectra acquired in similar conditions is a valuable strategy to mitigate this issue.

In order to assess how many spectra should be averaged for reaching the required SNR, we first evaluate the TROPOGAS noise.

As for the linearity assessment, the quartz-iodine lamp has been exploited. 50 quartz-iodine spectra have been measured with the same exposure time; thus, differences between the 50 measured spectra should have been due only to the noise but in reality, not null systematic differences sometimes exist. For this reason, the moving average over 15 points of the wavelength grid is subtracted to each measured spectrum in order to obtain 50 spectra with zero mean. It is still not clear the reason behind the systematic differences between quartz-iodine spectra acquired with same exposure times. Finally, for each point of the spectrum, the noise is computed as the standard deviation of the 50 zero-mean points of the different spectra.





In this way, we estimated the noise for each point of the wavelength grid that corresponds to a certain value (in counts) of quartz-iodine spectrum.

We applied this procedure to quartz-iodine spectra measured at two different spectral windows centered at 435.8 nm and 385 nm.

Figures 6 show that the results are equivalent in both the spectral windows (see black and blue dots). The noise increases with the spectra counts, from 20 in the part of the spectrum below 10000 counts to 90 where the spectrum counts reach 60000 (figure 6 on the left).

Since the noise increases slower than linearly, also the SNR increases with spectra counts from 200 to 700 (figure 6 on the right).

The exact number of spectra that should be averaged, for reaching the required SNR, will be assessed in the next future when the new measurement strategy, according to the FRM4DOAS operational guidelines, will be implemented.



Figure 6: Noise (left) and SNR(right) as function of spectrum counts, estimated in two spectral windows centered at 385 nm (black) and 435.8 nm (blue).

3.2.3 Example of TROPOGAS netCDF Level-1 file

After that spectra are acquired (according to the operational guidelines in section 3.2.2.2), they are processed (according to the data processing guidelines in section 3.2.2.3) and saved in netCDF format. In each netCDF file, all the level 1 data measured in a certain day and in a certain spectral window, are stored.

For example, the file named "BLQ01_20210211_4358.nc" contains all the spectra acquired by TROPOGAS during 11 February 2021 in the spectral window centered at 435.8 nm. Every file contains a title, a source, the channel, the instrument type, institution and dimensions information. Within every file, there are 2 groups named: "INSTRUMENT_LOCATION", and "RADIANCE". Inside the "INSTRUMENT_LOCATION" group, all geographical information variables, regarding the measurements site, are stored. The "RADIANCE" group contains two more groups named: "GEODATA" and "OBSERVATIONS". The variables that contain information about the viewing and solar zenith and azimuth angles are stored inside the "GEODATA" group, while the "OBSERVATION" group contains the atmospheric spectra with all the relative information. For more details, see table 1.





Variables in group "INSTRUMENT_LOCATION"

Name	Dim	Unit	Description	Example
Altitude (float32)	1	m	Altitude of the instrument above sea level	65
Latitude (float32)	1	degree_north	Latitude of the instrument (positive north)	44.52°
Longitude (float32)	1	degree_east	Longitude of the instrument (positive east)	11.42°
Altitude_of_station (float32)	1	m	Altitude of the station above sea level	50

Variables in group "RADIANCE/GEODATA"

Viewing_elevation_angle (float32)	Number_of_records	degree	Viewing elevation angle (0° is the horizon)	90°
Viewing_azimuth_angle (float 32)	Number_of_records	degree	Viewing azimuth angle 0360, measured towards the east, from north	0°
Solar_zenith_angle (float32)	Number_of_records	degree	Solar zenith angle (0° is the zenith)	30°
Solar_azimuth_angle (float32)	Number_of_records	degree	Solar azimuth angle 0360, measured towards the east, from north	170°

Variables in group "RADIANCE/OBSERVATIONS"

Wavelength (float32)	(number_of_records,detector_size)	nm	Wavelength grid	[440,440.06,]
Radiance (float32)	(number_of_records,detector_size)	counts	spectra	[30000,]
radiance_qflag (int16)	(number_of_records,detector_size)	//	Good value (1) Bad value (0)	[1,]
exp_time (float32)	number_of_records	S	Exposure time for the measured spectrum	4
number_of_coadded_spectr a (int16)	number_of_records	//	Number of averaged spectra	10
Datetime (int16)	(number_of_records,datetime_size)	//	Day and time info	[2021,02,03,11 ,12,00,00]
measurement_type (int16)	number_of_records	//	invalid (0) off-axis (1)	3



 Table 1: variables stored in netCDF files. The example in the right column refers to a zenith spectrum

 acquired during 03/02/2021 at 11:12.

4 Conclusions

In this document, we have presented the features of the TROPOGAS spectrometer that measures zenith and off-axis diffuse solar spectra since July 2018, over Bologna. In particular, its features have been compared to the FRM4DOAS standards and solutions have been proposed in order to achieve the highest possible number of compliant characteristics. According to the solutions adopted and described in section 3.2.2, TROPOGAS meets all the FRM4DOAS requirements except the FOV amplitude, as table 2 shows. The estimated TROPOGAS FOV has an amplitude of 3.6° (see 3.2.2.1) against 1.5° required by FRM4DOAS standards. In the next future, we plan to understand the impact of the FOV amplitude, by means of radiative transfer simulations, in MAX-DOAS measurements and consequently in the retrieved trace gases vertical profiles, with the aim to mitigate as much as possible the related effects.

Instrumental guidelines	
At least one O4 band covered well	V
Quartz fiber for removal of polarization features	V
Optical low pass filter for straylight removal in UV	V
Proper time information	V
Spectral resolution better than 0.8 nm (UV) and 1.5 (visible)	V
FOV better than 1.5° in vertical direction	X
Operational guidelines	
SZA range up to 85° for MAX-DOAS and up to 94° for zenith-sky observations	V
Zenith-sky observations at least every 30 minutes during MAX-DOAS observations	V





At least one zenith-sky measurement per degree SZA at twilight	V
At least 1°, 2°, 3°, 5°, 10°, 30° elevations in scan	V
Horizon scan on a regular basis	V
Dark signal must be measured at least daily	V
The slit function must be measured on a regular basis (daily if possible)	V
Data processing guidelines	
Apply dark signal correction	V
Apply wavelength calibration	V
Apply non-linearity correction	V
Average spectra to reach SNR of at least 3000 (visible) or 4000 (UV)	V

Table 2: list of all the FRM4DOAS requirements, met by TROPOGAS (green sign) and not (red sign).

5 References

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