Product Traceability and Uncertainty for the ground-based NDACC/FTIR O_3 profile product

Version 3

GAIA-CLIM
Gap Analysis for Integrated
Atmospheric ECV Climate Monitoring
Mar 2015 - Feb 2018

A Horizon 2020 project; Grant agreement: 640276

Date: 22 Dec 2017

Dissemination level: PU

Work Package 2; Complied by Matthias Schneider (IMK)

Table of Contents

Version history

Version	Principal updates	Owner	Date
0 draft	First draft	IMK	13.12.2017
1 draft	Minor changes by TG (NPL)	IMK	19.12.2017
2 draft	Minor changes by MS (IMK)	IMK	22.12.2017
3 draft	Minor changes following PT comments	IMK	11.01.2018

1. Product overview

Product name: Ground-based NDACC/FTIR O_3 profile product
Product technique: Remote sensing based on high resolution infrared solar absorption spectrometry
Product measurand: vertical distribution of tropospheric and stratospheric O_3.
Product form/range: from ground to about 50km.
Product dataset: MUSICA ground-based NDACC/FTIR dataset
Site/Sites/Network location: Kiruna (67.8°N, 20.4°E, 420 m a.s.l.) and Izaña (28.3°N, 16.5°W, 2370 m a.s.l.).

1.1 Guidance notes

This document describes the traceability and uncertainty for ground-based FTIR profile measurements of O_3. This product closely follows that out in the PTU document for MUSICA H_2O profile measurements and should be read in conjunction with that document.

2. Introduction

See PTU document for MUSICA H_2O profiles for a general introduction.

Specific for O_3:
The O_3 retrievals are performed in 5 spectral microwindows between 991 and 1014 cm^{-1}. Please note that here we report the data product as available via the NDACC database. It should be mentioned that an O_3 product retrieved by a simultaneous temperature fit would have significantly reduced random uncertainties due to improvement in the temperature profile used in the fit and reduced uncertainties in the temperature dependence of the spectroscopic line parameters (Schneider and Hase, 2008; García et al., 2012).

3. Instrument description

See PTU document for MUSICA H_2O profiles.

4. Product Traceability Chain

The product traceability chainis the same as shown in the PTU document for MUSICA H_2O profiles (Fig. 5 in the PTU document for MUSICA H_2O profiles). The following uncertainty contributors will be considered:

Uncertainty contributors from the measurement chain:
- A1: White noise in the measured spectral radiances (measurement noise)
- A2: Spectral baseline distortions (due to intensity fluctuations, detector non-linearities

and multi-reflections on optical elements)

Uncertainty contributors from the processing chain:
- B1: Line of sight/Pointing
- B2: Instrumental line shape (modulation efficiency and phase error)
- B3: Spectroscopic parameters and parameterisations
- B4: Solar spectroscopy
- B5: Atmospheric temperature profile assumptions

For details see PTU document for MUSICA H_2O profiles.

Figure 1 shows a typical averaging kernel for the ground-based FTIR O_3 profile product at Izaña.

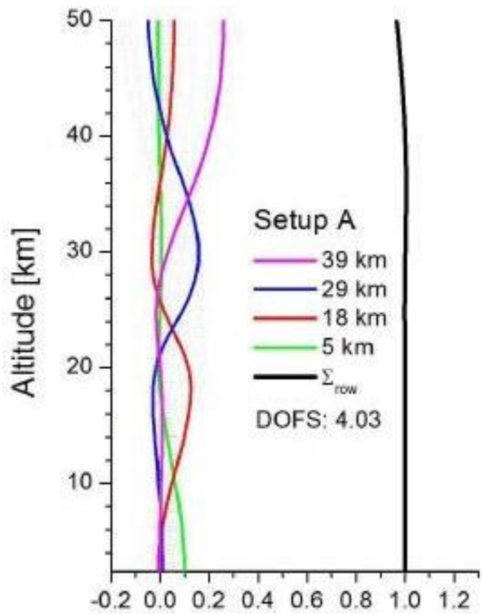

Figure 1. Logarithmic scale averaging kernel for a typical Izaña O_3 profile product (Graphic is adopted from Fig.2 of García et al., 2012). The green, red, blue and pink lines depict the response of the retrieved profile on real atmospheric O3 increases at 5, 18, 29, and 39km altitude, respectively. The black line is the sum along the row of the kernels and represents the sensitivity of the remote sensing system.

5. Element contributions

Here only the tables are given. For more general details please see the PTU document for MUSICA H_2O profiles.

5.1 Measurement noise (A1)

The measurement noise uncertainty contribution is taken from the root-mean-square value of the spectral fit residual (difference between measured and simulated spectrum). This kind of measurement noise includes white noise, but also systematic deficiencies in the forward simulations (error in spectroscopic parameters or parameterisations), an insufficient instrumental line shape description or spectral baseline distortions.

Information / data	Type / value / equation	Notes / description
Name of effect	Measurement noise	
Contribution identifier	A1	
Measurement equation parameter(s) subject to effect	Vector y in Eq. (3) of the PTU document for MUSICA H_2O profiles.	In addition the gain matrix **G**, because the actual noise level is for constraining the inversion process**.**
Contribution subject to effect (final product or sub-tree intermediate product)	Retrieved state vector $\hat{x}$	
Time correlation extent & form	None	No time correlation, however amplitude of noise can vary between different periods (e.g., by degradation of optical elements, see example of Fig. 8 of the PTU document for MUSICA H_2O profiles)
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units	< 1%, unitless (residual-to-signal ratio)	Typical ratio for retrievals using five microwindows in the 991-1014 cm^{-1} spectral range.
Sensitivity coefficient	Uncertainty propagation according to Eq. (9) of the PTU document for MUSICA H_2O profiles	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	The residuals.	It is not an absolute uncertainty instead it is a relative uncertainty, i.e. the residual is traceable relative to the signal.
Validation	Yes, by analysing the residuals.	

5.2 Spectral baseline distortions (A2)

Information / data	Type / value / equation	Notes / description
Name of effect	Baseline distortions	
Contribution identifier	A2	
Measurement equation parameter(s) subject to effect	Affects vector *y* in Eq. (3) of the PTU document for MUSICA H_2O profiles.	If known it could be considered in *F*(*x*,*p*). Then it would also affect the gain matrix **G** and the Jacobian matrix **K** in Eq. (3).
Contribution subject to effect (final product or sub-tree intermediate product)	Retrieved state vector $\hat{x}$	
Time correlation extent & form	Structured random	It is usually due to an instrumental/hardware problem, that will remain as long as it is not corrected.
Other (non-time) correlation extent & form		
Uncertainty PDF shape	The assumption is: 50% random (normal) and 50% systematic.	
Uncertainty & units	0.2% (chanelling-to-signal ratio), unitless 0.3% (offset-to-signal ratio), unitless	
Sensitivity coefficient	Uncertainty propagation according to Eqs. (7) and (8) of the PTU document for MUSICA H_2O profiles	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …		It is a relative uncertainty, i.e. it is traceable relative to the signal.
Validation	Laboratory measurements, e.g. Hase (2000).	

5.3 Line of Sight (LOS) / Pointing (B1)

Information / data	Type / value / equation	Notes / description
Name of effect	Pointing stability	
Contribution identifier	B1	
Measurement equation parameter(s) subject to effect	Affects vector function $F(x,p)$, the gain matrix $\mathbf{G}$ and and the Jacobian matrix $\mathbf{K}$ in Eq. (3) of the PTU document for MUSICA H_2O profiles.	
Contribution subject to effect (final product or sub-tree intermediate product)	Retrieved state vector $\hat{x}$	
Time correlation extent & form	Some time correlation possible (see Fig. 9) of the PTU document for MUSICA H_2O profiles.	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Assumption: 90% of the uncertainty to be random (normal) and the resting 10% of the uncertainty to be systematic.	
Uncertainty & units	0.001 rad = 0.0573°	
Sensitivity coefficient	Uncertainty propagation according to Eqs. (7) and (8) of the PTU document for MUSICA H_2O profiles	
Correlation(s) between affected parameters	Affect the retrieved state vector $\hat{x}$ in the same direction over all altitudes.	García et al. (2012)
Element/step common for all sites/users?	Yes	
Traceable to …	Qualitatively traceable to solar line frequency shifts (see Fig. 9 of of the PTU document for MUSICA H_2O profiles.)	
Validation	Possible, see example and discussion of Fig. 9 of the PTU document for MUSICA H_2O profiles.	

5.4 Instrumental line shape (B2)

At Kiruna and Izaña low pressure gas cell measurements are made regularly and wllo the determination of the modulation efficiency and the phase error within an uncertainty of smaller than 1% and 0.01 rad (see Fig. 10 of the PTU document for MUSICA H_2O profiles).

Information / data	Type / value / equation	Notes / description
Name of effect	Instrumental line shape (ILS)	
Contribution identifier	B2	
Measurement equation parameter(s) subject to effect	Affects vector function $F(x,p)$, the gain matrix **G** and and the Jacobian matrix **K** in Eq. (3) of the PTU document for MUSICA H_2O profiles.	
Contribution subject to effect (final product or sub-tree intermediate product)	Retrieved state vector $\hat{x}$	
Time correlation extent & form	Likely	See example of Fig. 10 of the PTU document for MUSICA H_2O profiles.
Other (non-time) correlation extent & form		
Uncertainty PDF shape	Assumption: 50% of the uncertainty to be random (normal) and the other 50% to be systematic.	
Uncertainty & units	Modulation efficiency is unitless (assumed uncertainty is 0.01) and the phase error unit is rad (assumed uncertainty is 0.01 rad)	
Sensitivity coefficient	Uncertainty propagation according to Eqs. (7) and (8) of the PTU document for MUSICA H_2O profiles	
Correlation(s) between affected parameters	Causes positive errors in the retrieved state vector $\hat{x}$ for certain altitudes that are correlated to negative errors at other altitudes (error patterns).	García et al. (2012)
Element/step common for all sites/users?	Yes	

Traceable to …	Hase (2012)	Modulation efficiency is a relative measurement, e.g. modulation efficiency at maximal optical path difference is related to the modulation efficiency at zero optical path difference.
Validation	Possible, like in Fig. 10 of the PTU document for MUSICA H_2O profiles. However, the sensitivity of these ILS retrievals has to be documented (like in Fig. 11 of the PTU document for MUSICA H_2O profiles.)	

5.5 Spectroscopic parameters and parameterisations (B3)

Information / data	Type / value / equation	Notes / description
Name of effect	Spectroscopy	
Contribution identifier	B3	
Measurement equation parameter(s) subject to effect	Affects vector function $F(x,p)$, the gain matrix $\mathbf{G}$ and and the Jacobian matrix $\mathbf{K}$ in Eq. (3) of the PTU document for MUSICA H_2O profiles.	
Contribution subject to effect (final product or sub-tree intermediate product)	Retrieved state vector $\hat{x}$	
Time correlation extent & form	Systematic	It is a systematic uncertainty
Other (non-time) correlation extent & form		
Uncertainty PDF shape	Normal	
Uncertainty & units	Uncertainty of 2% for the line intensity parameter (absolute unit for line intensity parameter is $cm^{-1}/(mol\ cm^{-2})$: Uncertainty of 5% for the pressure broadening parameter (absolute unit	Furthermore, the might be uncertainties by using an inadequate line shape model (see Fig. 12 of the PTU document for MUSICA H_2O profiles).

	for pressure broadening parameter is cm^{-1} / atm^{-1})	
Sensitivity coefficient	Uncertainty propagation according to Eqs. (7) and (8) of the PTU document for MUSICA H_2O profiles	
Correlation(s) between affected parameters	Causes positive errors in the retrieved state vector $\hat{x}$ for certain altitudes that are correlated to negative errors at other altitudes (error patterns).	García et al. (2012)
Element/step common for all sites/users?	Yes.	
Traceable to …		The inconsistency between the uncertainty of line parameters or parameterisations can be visualised in the differences between simulations and measured high-resolution, high quality spectra (see Fig. 12 of the PTU document for MUSICA H_2O profiles)
Validation		

5.6 Solar spectroscopy (B4)

Information / data	Type / value / equation	Notes / description
Name of effect	Solar lines	
Contribution identifier	B4	
Measurement equation parameter(s) subject to effect	Affects vector function $F(x,p)$, the gain matrix **G** and and the Jacobian matrix **K** in Eq. (3) of the PTU document for MUSICA H_2O profiles.	
Contribution subject to effect (final product or sub-tree intermediate product)	Retrieved state vector $\hat{x}$	
Time correlation extent & form	Structured random, similar to B1	

Other (non-time) correlation extent & form		
Uncertainty PDF shape	Assumption: 80% random (normal) and 20% systematic.	García et al. (2012)
Uncertainty & units	Solar line intensity: 1% uncertainty. Solar line ν-scale (Δν/ν): 10^{-6} uncertainty	García et al. (2012)
Sensitivity coefficient	Uncertainty propagation according to Eqs. (7) and (8) of the PTU document for MUSICA H_2O profiles	
Correlation(s) between affected parameters		
Element/step common for all sites/users?	Yes	
Traceable to …		
Validation	Solar line ν-scale can be validated according to Fig. 9 of the PTU document for MUSICA H_2O profiles.	

5.7 Atmospheric temperature profile assumptions (B5)

Information / data	Type / value / equation	Notes / description
Name of effect	Temperature	
Contribution identifier	B5	
Measurement equation parameter(s) subject to effect	Affects vector function $F(x,p)$, the gain matrix $\mathbf{G}$ and and the Jacobian matrix $\mathbf{K}$ in Eq. (3) of the PTU document for MUSICA H_2O profiles.	
Contribution subject to effect (final product or sub-tree intermediate product)	Retrieved state vector $\hat{x}$	
Time correlation extent & form	Possible.	Could occur if reanalyses data have systematic uncertainties.
Other (non-time) correlation extent & form	Possible.	Correlation between different sites are possible of the reanalysis data have correlated uncertainties

		between different sites.
Uncertainty PDF shape	Assumption: 70% random (normal) and 30% systematic.	
Uncertainty & units	Independently for three altitude ranges: surface – 10km: 1 K 10km – 37km: 2 K 37km – top of atmosphere: 5 K	
Sensitivity coefficient	Uncertainty propagation according to Eqs. (7) and (8) of the PTU document for MUSICA H_2O profiles	
Correlation(s) between affected parameters	Similar to B2 and B3 error patterns can occur.	
Element/step common for all sites/users?	Yes	
Traceable to …	None	
Validation	None	

6. Uncertainty Summary

Table 1. Uncertainty Summary.

Element identified	**Contribution name**	**Typical uncertainty value**	**Effect on final product (error of $\hat{x}$): T: troposphere S: stratosphere**	**Traceability level: L/M/H**	**Type**	**Correlated to**
A1	Noise	<1%	<0.5% (T) <0.2% (S)	H	100% random	A2, B2, B3
A2	Baseline	0.2% and 0.3%	<0.5% (T) <5% (S)	M	50% random and 50% systematic	A1
B1	Pointing	0.0573°	<0.03%	H	90% random and 10% systematic	B4
B2	ILS	1% and 0.01 rad	1.2% (T) 1.8% (S)	H	50% random and 50% systematic	A1
B3	Spectroscopy	2% and 5%	<10% (T) <7.5% (S)	L	100% systematic	A1
B4	Solar Lines	1% and 10^{-6}	<0.01%	M	80% random and	B1

					20% systematic	
B5	Temperature	1-5 K for 3 independent layers	<1% (T) <3% (S)	L	70% random and 30% systematic	None

7. Traceability uncertainty analysis

Traceability level definition is given in Table 2.

Table 2. Traceability level definition table

Traceability Level	Descriptor	Multiplier
High	SI traceable or globally recognised community standard	1
Medium	Developmental community standard or peer-reviewed uncertainty assessment	3
Low	Approximate estimation	10

Analysis of the summary table would suggest the following contributions, shown in Table 3, should be considered further to improve the overall uncertainty of the O_3 profile product. The entries are given in an estimated priority order.

Table 3. Traceability level definition further action table.

Element identifier	Contribution name	Typical uncertainty value	Effect on final product (error of $\hat{x}$): T: troposphere S: stratosphere	Traceability level: L/M/H	Type	Correlated to
B3	Spectroscopy	2% and 5%	<10% (T) <7.5% (S)	L	100% systematic	A1
B5	Temperature	1-5 K for 3 independent layers	<1% (T) <3% (S)	L	70% random and 30% systematic	None
A2	Baseline	0.2% and 0.3%	<0.5% (T) <5% (S)	M	50% random and 50% systematic	A1

1.1 Recommendations

In order to further improve the traceability of the O_3 profile products three priorities have been identified.

Similar to the MUSICA H_2O profile product also for the O_3 profiles the top priority is to quantify rigorously the uncertainty of the simulated spectroscopic signatures (contributor B3). In the meanwhile the measured spectra are of such high quality (low noise levels, high spectral resolution) that small uncertainties in spectroscopic parameters can have a significant effect on the product quality.

Second priority is the better quantification of the atmospheric temperature uncertainty (contributor B5). This should be characterised individually for each individual site in collaboration with providers of reanalyses data that are used as the atmospheric temperature in retrievals (NCEP). However, it should also be mentioned that by a simultaneous fit of the temperature profile this uncertainty contribution would be strongly reduced (Schneider and Hase 2008; García et al., 2012).

A better characterisation of the baseline distortions for each station individually (contributor A2) would also be recommendable. This might be achieved by performing regular analyses of black body radiances by the whole observing system (solar tracker unit and FTIR spectrometer). However, such calibration measurements can hardly be automated and would need more manpower.

In addition to improved assessment of the key uncertainty contributors described above further work could be undertaken to quantify and assess the nature of the uncertainties from the other (assumed minor) contributors from the other elements identified in the overall product traceability and uncertainty chain (see Fig.6 in MUSICA H_2O PTU document).

8. Conclusions

The ground-based NDACC/FTIR O_3 profile product for Izaña and Kiruna has been assessed against the GAIA CLIM traceability and uncertainty criteria.

9. References

García et al. (2012), doi:10.5194/amt-5-2917-2012.
Hase (2000), Dissertation, FZK Report No. 6512, Forschungszentrum Karlsruhe, Germany.
Hase (2012), doi:10.5194/amt-5-603-2012.
Schneider and Hase (2008), doi:10.5194/acp-8-63-2008.