Uncertainty Assessment for the measurement capabilities provided to WP5

A Horizon 2020 project;
Grant agreement: 640276
Date: 14th December 2016
Lead Beneficiary: BKS
Nature: R
Dissemination level: PU

Work-package	**WP2 (Measurement uncertainty quantification)**
Deliverable	D2.3
Nature	R
Dissemination	PU
Lead Beneficiary	BK Scientific GmbH, Mainz, Germany
Date	12/12/2016
Status	Final
Authors	Karin Kreher (BKS), Arnoud Apituley (KNMI), William Bell (MO), Matthias Buschmann (UBremen), Fabien Carminati (MO), Domenico Cimini (CNR), Francois Hendrick (BIRA), Jonathan Jones (MO), Bavo Langerock (BIRA), Fabio Madonna (CNR), Kalev Rannat (TUT), Peter Thorne (NUIM)
Editors	Peter Thorne (NUIM), Corinne Voces (NUIM)
Reviewers	Richard Davy (NERSC)
Contacts	karin.kreher@bkscientific.eu
URL	http://www.gaia-clim.eu

This document has been produced in the context of the GAIA-CLIM project. The research leading to these results has received funding from the European Union's Horizon 2020 Programme under grant agreement n° 640276. All information in this document is provided "as is" and no guarantee or warranty is given that the information is fit for any particular purpose. The user thereof uses the information at its sole risk and liability. For the avoidance of all doubts, the European Commission has no liability in respect of this document, which is merely representing the authors' view

Document history

Version	Author(s) / Reviewers	Date	Changes
0.1	Karin Kreher	08/12/16	Description of the uncertainty information of data streams identified within WP2 as likely data products to be included into the VO
0.2	Karin Kreher Peter Thorne Corinne Voces	12/12/16	Review of main text and addition of shortened questionnaires
Final	Karin Kreher Peter Thorne	13/12/16	Final review

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1. Document rationale and broader context

The purpose of this document is to provide background information for, and input to, the Virtual Observatory (VO) developed within WP5 on the measurement series from non-satellite sources which are to potentially be included. The VO facility will provide users with access to satellite and non-satellite data for comparison studies. A range of visualisation and analysis tools will be provided to explore and interact with the data. The non-satellite data sets under consideration to be provided to the VO are primarily being developed by WP2 Task 2.1 and the relevant subtasks, each one being instrument specific, with some additional data streams being provided by third party projects and reviewed by WP2 participants. To enable the VO user to adequately interpret and utilise these data sets within the Virtual Observatory, the necessary information regarding the suborbital measurements needs to be provided to WP5.

This exercise is carried out by WP2 whose main objective is the assessment of the measurement capabilities and uncertainty quantification of the investigated data series, and hence the qualification of the data series suitable for inclusion into the VO. The results are presented in this report (D2.3). The information needs to be made available to the VO development team in such a way that it can be implemented in fact sheets and/or interactive tools to enable user discovery and exploitation of the measurement series information. To provide the information in a consistent manner, a questionnaire previously developed and used within the FP7 project QA4ECV has been slightly modified for our purpose. This similarity between the templates enables cross-comparisons of outputs and potential exploitation of outcomes across the projects by end-users as well as participants in each project. The only key change made to the QA4ECV template is the addition of a section on measurement traceability and comparability.

2. Introduction to the questionnaire

The main sections included in the questionnaire in support of a comprehensive interpretation of each measurement technique are as follows:

1. **Identification of respondent and of data product**.
2. Short list of **Recommended literature.**
3. Description of **Main measured quantity (measurand).** This includes the specification of the measurand and the measurement equation (if available) describing the relation between the main measured quantity of the data product and any input quantities.
4. The **traceability and comparability** section describes if the measurement quantity is traceable to SI units or community accepted standards, and if and how comparability between measurements made at different sites is achieved.

5. **Representation of the uncertainty in the data product** lists the uncertainty field names and briefly describes the uncertainty form such as standard uncertainty (i.e. uncertainty expressed as standard deviation).
6. The **Uncertainty calculation** section provides information on how the uncertainty is calculated and the level of approximation used in these calculations.
7. The **Uncertainty contributions** section lists the main contributions to the uncertainty calculations such as a contribution introduced by the choice of prior, smoothing error, and noise. The section also describes if "random", "structured random" and "systematic" contributions are considered separately and if so, how each of them are defined in the uncertainty calculations. This section further covers if the data product depends on input quantities and how the final uncertainties then depend on the uncertainties of the input quantities, and finally on the information on uncertainties due to model error.
8. This section deals with the presence of **Correlations/covariances** in the data product. It also identifies and documents any auto-correlation and correlation between the main measured quantity and other quantities.
9. **Bias handling introduced during processing** and if this is corrected for.
10. **Other remarks on data product uncertainty**

The GAIA-CLIM questionnaire was distributed to the appropriate instrument experts within WP2 and the broader GAIA-CLIM project consortium and the completed questionnaires are collated in Annexes A through O of this report as detailed in Table 1. In a couple of cases, where the instrument and measurement technique expertise was not fully available within GAIA-CLIM, input from the wider science community was invited to review limited aspects of the completed draft questionnaire prior to finalisation.

Annex	Instrument	ECV(s)	Primary compiler
A	Lidar	Aerosols	CNR
B	Lidar	Water vapour profiles	KNMI
C	Lidar	Ozone profiles	KNMI
D	Lidar	Temperature profiles	KNMI
E	Microwave radiometer (MWR)	Water vapour profiles	CNR
F	Microwave radiometer (MWR)	Temperature profiles	CNR
G	Microwave radiometer (MWR)	Total water vapour content (TWVC)	CNR

H	Microwave radiometer (MWR)	Total liquid water content (TLWC)	CNR
I	FTIR Spectrometer (NDACC)	FTIR NDACC O_3 and CH_4 FTIR MUSICA H_2O	BIRA
J	FTIR Spectrometer (TCCON)	FTIR TCCON CO_2 and CH_4	UBremen
K	UV-visible spectrometer (DOAS)	Total ozone column	BIRA
L	Dobson	Total ozone column	BKS
M	GNSS	Total column water vapour	TUT
N	GRUAN RS92 radiosonde geophysical profiles	Temperature profile Humidity profile	NIUM
O	GRUAN RS92 radiosonde radiance equivalents	Top-of-atmosphere (TOA) brightness temperatures	MO

Table 1. Summary of compiled questionnaires presented in the Annexes.

3. Data products

The following data products, highlighted in Table 1, have been selected within GAIA-CLIM as being potentially mature enough to be likely candidates for data streams of reference quality and hence to be considered for the inclusion into the VO. The traceability chains for the products discussed under 1)-3), 4) (for UV-vis only) and 5) as below are available on the GAIA-CLIM website (http://www.gaia-clim.eu/page/traceability-model-diagrams). The uncertainty assessment for the measurement capabilities has been completed by the relevant instrument experts within GAIA-CLIM with some guidance, where appropriate, from the wider community.

1) **Annex A-D:** Lidar measurements of aerosol, water profiles, ozone profiles and temperature profiles are either already ready to be included into the VO (in the case of ozone) or expected to be ready within the GAIA-CLIM project time-period. The lidar community has developed robust data processing procedures which include the estimation of the random uncertainty and a separate estimation of the systematic uncertainties due to a few retrieval assumptions, background models, and corrections implemented in a typical lidar data processing chain. In-depth literature is available and up-to-date.

2) **Annex E-H:** The 2nd group of data products chosen for potential inclusion into the VO are water vapour and temperature profiles, total water vapour content and total liquid water content measured with microwave radiometer (MWR). The literature sources provided in the questionnaires for the MWR products are up-to-date and the uncertainties in MWR

products are provided by the ARM Program (Atmospheric Measurement Program, www.arm.gov) and by the HD(CP)2 project (High Definition Clouds and Precipitation for Climate Prediction, https://hdcp2.zmaw.de). Uncertainties in MWR derived products are usually estimated *ex ante* through simulated analysis and/or *ex post* through validation against collocated radiosonde profiles.

3) **Annex I-J:** Ozone and methane profiles measured by FTIR under the umbrella of NDACC (Network for the Detection of Atmospheric Composition Change), TCCON (Total Carbon Column Observing Network), and MUSICA H_2O. The measured quantity is an interferogram which is then Fourier transformed to an absorption spectrum in arbitrary units. From the shape of the absorption lines in selected micro-windows, information on targeted gas concentrations using optimal estimation can be deduced. The uncertainties are given as standard deviation and are reported as covariance matrices, containing correlations in the height axis. The literature sources provided in the questionnaires for the FTIR products are up-to-date.

4) **Annex K-L:** Total ozone columns retrieved from twilight ground-based DOAS UV-visible measurements and Dobson measurements are seen to be ready to be included in the VO. The literature sources provided in the questionnaires for the ozone products are up-to-date. The uncertainty budget on twilight UV-visible ozone columns is separated into random and systematic uncertainties for the three main retrieval steps (spectral fit, determination of the residual amount in the reference spectra and airmass factor extraction/calculation). For the Dobson uncertainties a table is provided with preliminary entries based on model calculations. A more realistic and comprehensive uncertainty budget, which will be tested with measurements from two measurement campaigns, is envisaged to be made available in October 2017. The corresponding traceability chain for the Dobson measurements has been developed in the framework of the WMO GAW Dobson network. Details on the uncertainty of Brewer measurements are also currently under review as part of the ATMOZ project which is addressing the traceability of atmospheric total column ozone specifically for Brewer and Dobson measurements with results expected to become available later in 2017.

5) **Annex M:** GNSS Total Column Water Vapour (TCWV) is derived from GNSS signal Zenith Total Delays (ZTD) by adding atmospheric and surface meteorological constraints and processing with dedicated software. The relationship between the main measured quantity of the data product and input quantities is indirect – the GNSS receiver can detect only GNSS signal delays on the ray path between an orbiting GNSS satellite and the ground-based receiver. Those delays with satellite orbital parameters and different physical constants will be inserted to a system of navigation equations and processed by geodetic software with one of the final products from GNSS data processing being ZTD. The

uncertainty in TCWV is traceable via an unbroken chain to the original time-delay measurement (the SI unit of seconds) and the product is ready to be implemented within the GAIA-CLIM project lifetime.

6) **Annex N:** The GRUAN RS92 radiosonde product undertakes a full metrological characterisation based upon lab, bench and field characterisation of the instrument. The analysis is fully traceable and the analysis is commensurate with the GUM practices and the VIM. Within the uncertainty calculation, typically there are several sources of uncertainty quantified for each measured parameter via a range of techniques. Each of these sources of uncertainty is derived experimentally and parameterised mathematically. For all measurements there exists a calibration uncertainty which is a perfectly correlated term within each measurement series profile.

7) **Annex O:** Top-of-atmosphere (TOA) brightness temperatures are simulated from GRUAN radiosonde measurements and NWP models using the approach being developed in GAIA-CLIM by WP4. This innovative approach establishes the uncertainties in simulated TOA brightness temperatures generated from NWP models. Although the GRUAN measurements themselves are fully traceable, the radiative transfer model which projects these into TOA brightness temperatures is based on spectroscopic parameters (linestrength, linewidths, and pressure broadening parameters) that are not yet fully traceable and the complete uncertainty procedure is still under development.

At the time of writing this document, it is unclear if ozone profiles measured by ozonesondes will be ready to be included as reference data set into the GAIA-CLIM VO with respect to full traceability of the uncertainty chain, and hence this data stream has not been included here. Similarly, at this stage, MAX-DOAS measurements of ozone are not envisaged to be included in the VO since it is unlikely that the full traceability chain covering all processing steps will be available within the GAIA-CLIM time frame. If either of these products end up being available for use within the VO then WP2 shall solicit questionnaire responses for these products and provide these to WP5 at a later date and the questionnaires shall also be hosted on the project webpage.

4. Summary

The collation of the questionnaires has provided a comprehensive overview of the status of the measurement uncertainties for the data streams under consideration to be included into the VO. The information gathered by the instrument experts within the individual questionnaires provides users of these data products with detailed and up-to-date information on the uncertainties, in most cases both with explicit descriptions within the questionnaire as well as with a list of the most relevant publications for additional and more in-depth information.

Furthermore, collating the uncertainty information for data streams measured with a variety of diverse techniques in a consistent manner helps to understand the differences between these data products. In particular for the data streams such as ozone which are measured with several techniques (lidar, FTIR, UV-vis spectroscopy, ozonesondes, etc.), the actual observed quantities and their uncertainties vary and a collation of this information in a consistent format fosters a more accurate understanding of the differences observed when comparing the same target species measured with a range of different instruments.

5. Annex A-O

All questionnaires are listed as Annex A – O with the first questionnaire (Annex A) in its complete form and all following ones without the introduction and glossary which is identical for all questionnaires. Each individual Annex (or questionnaire) has its own table of contents.

GAIA-CLIM

Questionnaire about uncertainty in data products

Date: October 2016

Lead Beneficiary: BKS

Nature: R

Dissemination level: PU

Grant agreement n°640276

Work-package	WP 2
Deliverable	D2.3
Title	Questionnaire about uncertainty in data products
Nature	R
Dissemination	PU
Lead Beneficiary	BKS
Date	14 December 2016
Status	Final
Authors	Karin Kreher (modified slightly from original used in FP7 project QA4ECV provided by BIRA-IASB colleagues with permission)
Editors	Peter Thorne
Reviewers	Arndt Meier
Contacts	karin.kreher@bkscientific.eu
URL	http://www.gaia-clim.eu

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Rationale and context

Within GAIA-CLIM, a Virtual Observatory (VO) is under development to enable end-users to visualize, interrogate, and download co-locations between satellite data and high-quality sub-orbital data to aid the characterization and validation of satellite missions. To this end, users shall require information regarding the sub-orbital measurement series to be able to properly interpret and utilise these data within this Virtual Observatory facility.

Work Package 2 is concerned with the qualification of measurement series suitable for inclusion within the Virtual Observatory. As part of WP2, Deliverable 2.3 includes provision of necessary information about each measurement system identified to date as plausibly contributing to the Virtual Observatory. This information needs to be sufficient for the Virtual Observatory development team to be able to implement fact sheets and / or interactive tools to enable user discovery and exploitation of measurement series information.

This questionnaire will provide the necessary information to allow the development of user support tools by the Virtual Observatory team. The goal of this questionnaire is to provide a consistent template to the WP2 instrument experts so they can, in turn, provide the necessary information and documentation about the uncertainty on the main output quantities as provided in their data product in a consistent manner to the developers for subsequent implementation.

The questionnaire is a slight modification of a similar questionnaire performed under the FP7 project QA4ECV which considers a number of complimentary ECVs and measurement techniques. This similarity enables cross-comparisons of outputs and potential exploitation of outcomes across the projects by end-users as well as participants in each project.

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1. Identification of respondent and of data product

What are your contact details?

Answer:
Fabio Madonna
Consiglio Nazionale delle Ricerche - Istituto di Metodologie per l'Analisi Ambientale (CNR-IMAA)
C.da S. Loja
85050 Tito Scalo (Potenza)
Italy
Tel: +390971427252
Fax: +390971427271
Skype: fabio.madonna
E-mail: fabio.madonna@imaa.cnr.it
http:www.imaa.cnr.it
http://www.ciao.imaa.cnr.it

For which data product are you filling in this questionnaire?

Answer: Aerosol lidar optical properties (backscattering and extinction coefficient)

Please provide one or more accessible sources of information that a non-expert user can refer to, to gain an understanding of the measurement technique.

Answer:
Wandinger, U., 2005: Introduction to lidar. Lidar: Range-Resolved Optical Remote Sensing of the Atmosphere, C. Weitkamp, Ed., Springer Series of Optical Sciences, Vol. 102, Springer, 1–18.

2. Recommended literature

*Which literature work would you recommend to understand better the measurement technique and the **general uncertainty framework** within which uncertainties of the data product are constructed. Note that for metrology, the vocabulary list of the VIM (*International Vocabulary of Metrology, [RD18]*), and the uncertainty framework of the GUM (Guide to expression of uncertainty,* [RD4]*) are important standards. Please provide a complete reference or doi where possible.*

Answer:
Lidar community has developed over the years a robust data processing which includes the estimation of the random uncertainty and a separate estimation of the systematic uncertainties due to a few retrieval assumptions, background models, and corrections implemented in a typical lidar data processing chain. Nevertheless, this general framework, whose description can be found in the references reported in this section has been not always developed in a fully compliant way with the VIM and GUM. On other hand the refinement of the existing framework to make it fully complaint with the VIM and GUM looks not challenging and this results could be easily achieved in cooperation with the lidar community.

Wandinger, U., 2005: Introduction to lidar. Lidar: Range-Resolved Optical Remote Sensing of the Atmosphere, C. Weitkamp, Ed., Springer Series of Optical Sciences, Vol. 102, Springer, 1–18.

*More specifically, which literature works (article, ATBD, other…) would you recommend to understand better how uncertainties of **this particular data product** are conceived? Please provide a complete reference or doi where possible.*

Answer:

D'Amico, G., Amodeo, A., Mattis, I., Freudenthaler, V., and Pappalardo, G.: EARLINET Single Calculus Chain – technical – Part 1: Pre-processing of raw lidar data, Atmos. Meas. Tech., 9, 491-507, doi:10.5194/amt-9-491-2016, 2016.
Mattis, I., D'Amico, G., Baars, H., Amodeo, A., Madonna, F., and Iarlori, M.: EARLINET Single Calculus Chain – technical – Part 2: Calculation of optical products, Atmos. Meas. Tech., 9, 3009-3029, doi:10.5194/amt-9-3009-2016, 2016.

Please specify also if the literature source is still up-to-date with the current data product. If not, where can a user find the information on the latest version of the data product and its uncertainties?

Answer: Literature is up-to-date though this is in continuous evolution: for example a paper specifically for the discussion of the uncertainty on the retrieval of the lidar optical properties should be submitted in the AMT EARLINET special issue in 2017.

3. Main measured quantity (measurand)

3.1 Specification of measurand

Specify the main measured quantities (i.e., the measurands) and the associated unit of the data product, along with their field name in the data product

Example measurands with unit: Temperature [K], O3 profile [ppmv], water vapour [ppmv]

Quantity [unit]	Field name
Aerosol backscattering coefficient (m-1 sr-1)	Backscatter_coefficient

Aerosol extinction coefficient (m-1)	Extinction_coefficient

3.2 Measurement equation

What is the relation between the main measured quantity of the data product and input quantities? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to literature publications).

Answer:

The lidar equation is the way to relate the light power backscattered by the atmospheric target with the signal collected by the lidar receiver. In a general form, the lidar equation can be written as

$$P(\lambda_L,\lambda_S,z)=P_L(\lambda_L)\Psi(\lambda_S,\lambda_L)O(z)\beta(\lambda_S,\lambda_L,\theta,z)\frac{A}{z^2}\frac{c\tau_d}{2}\exp\left(-\int_0^z\alpha(z)dz\right)+P_B \qquad \text{[Eq.11]}$$

where:

$P(\lambda_L,\lambda_S,z)$ is the backscattered power received from the distance z from the source (zenith pointing), at a specific polarization and wavelength λ_s, due to the scattering of the laser wavelength λ_L;

$\Psi(\lambda_S,\lambda_L)=\xi(\lambda_L,\lambda_S)\eta(\lambda_S)$ is transmission of the lidar receiver, given by $\xi(\lambda_L,\lambda_S)$ that is the optical efficiency of the lidar receiver, including such factors as the reflectivity of the telescope and the transmission of the conditioning optics, while $\eta(\lambda_S)$ is the quantum efficiency of the receiver and detection parts;

$O(z)$ is the system overlap function;

$P_L(\lambda_L)$ is the output laser power at the wavelength λ_L;

$\beta(\lambda_S,\lambda_L,\theta,z)$ is the volume scattering coefficient at the distance z and at an angle θ and represents the probability that a transmitted photon is backscattered by the atmosphere into a unit solid angle ($\theta=\pi$);

$\frac{A}{z^2}$ is the probability that a scatter photon from the distance is collected by the receiving telescope of surface A;

$\frac{c\tau_d}{2}$ represents the sounding vertical resolution, where c and τ_d are respectively the light speed and the dwell time (i.e. the laser duration pulse);

$\exp\left(-\int_0^z\alpha(z)dz\right)$ is the two-way transmissivity of the light from laser source to the distance z and from distance z to the receiver, respectively;

P_B is the contribution power return due to the background photons.

To use of [Eq.11] for the inversion of the backscattered radiation and to retrieve the atmospheric parameters, the approximation of single and independent scattering is needed: this means that a photon is scattered only once by the atmospheric constituents and that these are separated adequately and are moving randomly. Thus, the contribution to the total scattered energy by many targets have no phase relation and the total intensity is simply the sum of the intensity scattered from each target.

A much broader description is available at:
http://cfa.aquila.infn.it/wiki.eg-climet.org/index.php5/Lidar_fundamentals
http://cfa.aquila.infn.it/wiki.eg-climet.org/index.php5/Raman_LIDAR_Fundamentals

Ansmann, A, M Riebesell, and C Weitkamp. Measurements of atmospheric aerosol extinction profiles with Raman lidar, Optics Letters 15:746-748, 1990.

Ansmann, A., Wandinger, U., Riebesell, M., Weitkamp, C., and Michaelis, W.: Independent measurement of extinction and backscatter profiles in cirrus clouds by using a combined Raman elastic-backscatter lidar, Appl. Optics, 31, 7113–7131, 1992.

Ferrare, R. A., S. H. Melfi, D. N. Whiteman, K. D. Evans, and R. Leifer, Raman lidar measurements of aerosol extinction and backscattering: 1. Methods and comparisons, J. Geophys. Res., 103, 19,663–19,672, 1998.

Fiocco, G.; and Smullin, L. D., (60-140 km) by Optical Radar. Detection of Scattering Layers in the Upper Atmosphere Nature I;ae, I275 (1963).

Klett, J. D., Stable analytic inversion solution for processing lidar returns, Appl. Opt., 20, 211–220, 1981.

4. Traceability and comparability

4.1 SI or community traceability

Is the measurement quantity traceable, via an unbroken chain of processing steps, to SI units or community accepted standards?

Answer:

The measurements quantities are traceable to community accepted standards which is represented by:

- For the elastic backscattering lidar by an estimated profile (from a model or from an in-situ sounding) of the molecular backscattering at each measured wavelength which is used as the reference for the calibration of lidar backscattering profile.
  Scattering from molecules is of major importance for lidar since the signal from the molecules can be used as a lidar calibration source. Lidar calibration is required for obtaining the system constant needed for particle backscattering coefficient profile retrievals. The conventional calibration approach is to normalize the lidar return to a given molecular reference value in the upper troposphere or stratosphere. This is challenging to apply in the near-IR because of the weak molecular scattering and, above all for ceilometers, of the low signal-to-noise ratio. Moreover, the uncertainty due to the use of a calibration value of the molecular scattering equal to zero (i.e. no aerosol scattering), that is often considered in the signal inversion, can be furthermore critical at infrared wavelengths (larger than 35%), while at lower wavelengths the uncertainty in much lower (within 10 %).
  The uncertainty due the molecular profile adopted for the calibration of lidar signals (based on radiosoundings profiles, weather forecast models, theoretical simulations) has been also estimated and quantified In a few percents.

- For a Raman/elastic lidar, the retrieval of the aerosol extinction profile is “autocalibrated”. Aerosol extinction can be retrieved with very low assumptions exploiting the significant

advantage coming from the use of Raman backscatter: this assumption is related to the spectral dependency of the extinction coefficient which is limited to less than 4% on the final retrieval. The backscattering coefficient is calibrated using the ratio at aerosol free altitude between two signals, one is the elastic backscattered signal and the other is the nitrogen Raman signal used as the reference of the molecular atmosphere.
Raman backscatter occurs when the scattering molecules transit from one energy state to another before reemitting the incident light. This results in scattering at shifted frequency/ wavelength equal to the difference (the combination) of the incident light frequency and the frequency gap between the final and the initial energy states of scattering molecules. The frequency/wavelength shift depends on the transition type and has a different value for different types of scattering molecules (Serikov et al., 2009). The fraction of the total energy scattered at that wavelength (i.e., the Raman cross-section) is typically three orders of magnitude smaller than for elastic scattering, which allows its practical application to remote sensing of only the most abundant molecules in the atmosphere, like nitrogen or water vapor.

If yes, please provide references to available literature describing the traceability aspects of the measurement.

Ansmann, A, M Riebesell, and C Weitkamp. Measurements of atmospheric aerosol extinction profiles with Raman lidar, Optics Letters 15:746-748, 1990.

Wandinger, U., 2005: Introduction to lidar. Lidar: Range-Resolved Optical Remote Sensing of the Atmosphere, C. Weitkamp, Ed., Springer Series of Optical Sciences, Vol. 102, Springer, 1–18.

Di Girolamo, P., P. F. Ambrico, A. Amodeo, A. Boselli, G. Pappalardo, and N. Spinelli, Aerosol observations by lidar in the nocturnal boundary layer, Appl. Opt., 38(21), 4585–4595, 1999.

If no, please describe what aspects of the measurement are not fully traceable and how this aspect is addressed in deriving the data product and its uncertainty.

4.2 Comparability

If measurements are taken at multiple sites, are efforts made to ensure sufficiently similar measurement technique approaches to ensure comparability? Please provide links to any supporting materials available such as instrument manuals / network protocols.

Answer:
A comprehensive strategy for campaign setup and data evaluation has been established at European level. Eleven systems from nine EARLINET stations participated in the EARLINET Lidar Intercomparison 2009 (EARLI09). In this campaign, three reference systems were qualified which served as traveling standards thereafter. EARLINET systems from nine other stations have been compared against these reference systems since 2009; afterwards the systems have calibrated other instrument travelling from their own station to the other sites in the various countries.
A strategy for ensuring the lidar system comparability at the global is currently missing. GALION (GAW Lidar Observation Network) is the global federation of lidar networks operating in the

different continents: the network implementation is challenging and its collective operation is limites to special events (Sawamura et al., 2012), lilke volcanic eruptions. Neverthleess, the lidar calibration facility (LICAL) active in the frame of ACTRIS2 H2020 research infrastructure project offers to calibrate all lidar system types from outside the ACTRIS community with a special focus on GALION federated networks. In future LICAL could become the calibration center for a global network.

Wandinger, U., Freudenthaler, V., Baars, H., Amodeo, A., Engelmann, R., Mattis, I., Groß, S., Pappalardo, G., Giunta, A., D'Amico, G., Chaikovsky, A., Osipenko, F., Slesar, A., Nicolae, D., Belegante, L., Talianu, C., Serikov, I., Linné, H., Jansen, F., Apituley, A., Wilson, K. M., de Graaf, M., Trickl, T., Giehl, H., Adam, M., Comerón, A., Muñoz-Porcar, C., Rocadenbosch, F., Sicard, M., Tomás, S., Lange, D., Kumar, D., Pujadas, M., Molero, F., Fernández, A. J., Alados-Arboledas, L., Bravo-Aranda, J. A., Navas-Guzmán, F., Guerrero-Rascado, J. L., Granados-Muñoz, M. J., Preißler, J., Wagner, F., Gausa, M., Grigorov, I., Stoyanov, D., Iarlori, M., Rizi, V., Spinelli, N., Boselli, A., Wang, X., Lo Feudo, T., Perrone, M. R., De Tomasi, F., and Burlizzi, P.: EARLINET instrument intercomparison campaigns: overview on strategy and results, Atmos. Meas. Tech., 9, 1001-1023, doi:10.5194/amt-9-1001-2016, 2016.

5. Representation of the uncertainty in the data product

5.1 Uncertainty field name(s)

Which field name(s) are used in the data product to hold the uncertainty value(s) associated with the main measured quantities? Note that more than one uncertainty field name can be associated with a single quantity (e.g., one field name for the "uncertainty due to random effects" and one for the "uncertainty due to systematic effects").

Field name of uncertainty	Associated quantity
Error	Random uncertainty

5.2 Uncertainty form

In what form is the uncertainty per measurement represented in the data product? For example, is it:

- *A standard uncertainty (i.e., uncertainty expressed as standard deviation)*
- *A 95% coverage interval*
- *A variance-covariance matrix (if so, explain between which quantities the covariance is taken into account)*
- *A probability density function*
- *Other [please specify]*

Answer: Standard uncertainty (i.e., uncertainty expressed as standard deviation). All the other contribution to the uncertainty budget (due to the molecular profile used for the calibration or to the assumptions of a lidar ratio value of a single calibration value) can be derived from information reported into the data files but are not provide as variables with a specific field name.

6. Uncertainty calculation

6.1 Formula/procedure

What is the formula/procedure by which the uncertainty is calculated? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to one or more equations in the literature).

Answer:

Uncertainty on the extinction coefficient (random)

This is largely described in the EARLINET-ASOS report "Assessment report of existing calculus subsystems used within EARLINET-ASOS" available at http://wiki.tropos.de/images/7/7a/Subsystems.pdf, compiled by I. Mattis, A. Chaikovsky, A. Amodeo, G. D'Amico, and G. Pappalardo (April 1, 2007).

Uncertainty on the backscatter coefficient (random)

D'Amico, G., Amodeo, A., Mattis, I., Freudenthaler, V., and Pappalardo, G.: EARLINET Single Calculus Chain – technical – Part 1: Pre-processing of raw lidar data, Atmos. Meas. Tech., 9, 491-507, doi:10.5194/amt-9-491-2016, 2016.

Mattis, I., D'Amico, G., Baars, H., Amodeo, A., Madonna, F., and Iarlori, M.: EARLINET Single Calculus Chain – technical – Part 2: Calculation of optical products, Atmos. Meas. Tech., 9, 3009-3029, doi:10.5194/amt-9-3009-2016, 2016.

Is the uncertainty obtained by:

- *Uncertainty propagation, taking into account the uncertainties of the input quantities,*
- *Probability density function propagation,*
- *Sensitivity analysis: i.e., varying parameters and check the impact on the output quantity,*
- *Or still some other procedure?*

Answer: Two options are available: "Monte Carlo" error calculation and "error of the used method" (uncertainty propagation, taking into account the uncertainties of the input quantities). Details are reported in the above mentioned references. The two methods have been compared and are in pretty good agreement if a sufficient number of simulation is performed with the Monte Carlo method (minimum of 30).

6.2 Level of approximation

In what way is the uncertainty calculation procedure an approximation?

- *Is it based on (as is common practice) a first-order Taylor approximation (see GUM* [RD4], *Eq. (13))*

$$u_c^2(y) = \sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i, x_j) = \sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i, x_j)$$

which will not be exact if f is nonlinear.

- *Are correlations between input quantities neglected?*
- *Other approximations?*

Answer: Correlations between input quantities are neglected. Different error sources of the algorithm are assumed independent and uncorrelated, which is not strictly valid though it might be considered negligible in a first approximation. This is the case of gluing two lidar signals measured at the same wavelength but using different detection modes, for example. For the vertical smoothing of the aerosol profiles instead, which is mandatory for the retrieval of the extinction profiles (and for consistency also for the backscatter coefficient), a second-order low pass filter is typically applied acting on the final product or alternatively on the raw input signal. In this case, an effective resolution profile is provided along with the aerosol extinction and backscatter profiles which is the result of the correlation between the smoothed points.

If an approximation is involved, do you think the approximation can be a problem, or do you consider it justified?

Answer:
Any involved approximation is justified as a compromise between the limit of the applied measurement technique and its contribution to the total uncertainty budget. Some of the approximations are more critical, many other much less so. For the elastic retrieval the assumption typically made for retrieving the optical products can bias the retrieval by up to 50 %, while for the Raman and Raman/elastic retrieval the effect of the assumptions is limited to a few percent. For example, the uncertainty due to the use of a calibration value of the molecular scattering equal to zero (i.e. no aerosol scattering), that is often considered in the signal inversion, can be furthermore critical at infrared wavelengths (larger than 35%), while at lower wavelengths the uncertainty in much lower (within 10%). Similarly, for the uncertainty due to the assumption of a lidar ratio value for the elastic lidar retrieval, this can largely bias the retrieval by up to 50 % depending on the detection wavelength. This is less critical, for example, at the infrared wavelengths.

7. Uncertainty contributions

7.1 Prior

Is there a prior contribution? If so, is this prior based on measured data, a model, a rough guess, or something else?

Answer: Scattering from molecules used as a lidar calibration source can be calculated from air pressure and temperature profiles taken from radiosonde launches, from atmospheric models (e.g. US standard atmosphere), or analysis data sets of numerical weather prediction models. Absorption due to molecules is typically neglected for these wavelengths.

7.2 Smoothing error

Is an error source "smoothing error" included in the uncertainty calculation? If so, what do you define as "smoothing error"? Should the averaging kernel of the data product be applied in some way, before the uncertainty can be properly interpreted?

Answer: Yes, regarding the EARLINET network. In the last development of the EARLINET Single-Calculus-Chain (SCC), which is a centralized processing software for the lidar data analysis, each profile is accompanied by a profile indicating the effective vertical resolution which is the result of the applied smoothing filtering. The related covariance matrix is not provided but can be calculated from the smoothing data.

7.3 Noise

Is there a noise contribution? If so, what do you define as "noise"? (E.g., for MOPITT, one considers an instrumental noise, but also a "geophysical noise" (Deeter, 2013).)

Answer: Yes, this is due to the background noise measured on each single or integrated lidar signal before the processing, subtracted according to the solution of the lidar equation.
In addition, the noise due to dark currents (instrumental noise due to the electronics), which provides a sort bias on the collected signal in analog detection mode, is measured before or after each measurement session by obscuring the instrument receiver and is then subtracted from the measured signals during the signal processing.

7.4 Random and systematic contributions

Do you consider explicitly separately "random", "structured random" and "systematic" contributions? If so, how do you define each of these in your calculation?

Answer:

Main sources of uncertainties for the extinction retrieval are [Pappalardo et al., 2004]:

- the random error that is due to signal detection,
- the systematic error associated with the estimate of temperature and pressure profiles,
- the systematic error associated with the estimate of ozone profiles in the UV,
- the systematic error associated with the wavelength-dependence parameter å,
- the systematic error associated with multiple scattering,
- the error introduced by data-handling procedures such as signal averaging during varying atmospheric extinction and scattering conditions.
- largest extinction uncertainties are caused by the overlap function O(z) [Wandinger and Ansmann, 2002].

Main sources of uncertainties for the retrieval of the backscatter coefficient are:

- the random error due to signal noise, which is usually derived by means of error propagation,
- the systematic error associated with the estimate of temperature and pressure profiles, which has values of up to 1.5% [Masonis et al., 2002],
- the systematic error associated with the wavelength-dependence parameter å; this error is about 2%-5% for most atmospheric conditions.
- the error introduced by data-handling procedures such as signal averaging during varying atmospheric extinction and scattering conditions,
- the systematic error associated with the differential overlap function,
- the systematic error associated (up to 10%) caused by the assumption of a backscattering value in the calibration region [Ansmann et al., 1992a],
- the systematic error associated to the assumption of a particle lidar ratio (profile); this error can easily exceed 20% [Sasano et al., 1985].

7.5 Input quantities / other parameters

If the main measured quantities of the data product depend on input quantities, how do the final uncertainties depend on uncertainties of these input quantities? Please provide a list with input quantities of which the uncertainties:

1. *Are taken into account.*
2. *Could be important, but are not taken into account. For example, because their consideration would be technically difficult, or it is not clear how to estimate the associated uncertainty.*
3. *Are not taken into account, as they can be demonstrated to be negligible.*

If this list is already available somewhere in a literature source, you can simply refer to it.

Input quantity/other parameter	associated uncertainty or "important but ignored" or "negligible"	Extra info (e.g., random, systematic)
Lidar ratio	Important (decreases with the wavelength)	systematic
Calibration backscattering value	Important (increases with the wavelength)	systematic
Angstrom coefficient	negligible	systematic
Error associated with the estimate of temperature and pressure profiles	negligible	systematic

7.6 Uncertainty due to model error

Do you consider explicitly an uncertainty contribution due to the fact that the model is not perfect? Such uncertainty can be revealed e.g., by comparing results of several retrieval models.

Answer: See above the description at section 7.4 of the error associated with the estimate of temperature and pressure profiles.

8. Correlations/covariances

8.1 Presence in data product

Do you provide correlations or covariances within your data product, directly relevant to the main measured quantity? If so, between which quantities?

Answer: No. As mentioned above, each profile is accompanied by a profile indicating the effective vertical resolution which is the result of the applied smoothing filtering. The related covariance matrix is not provided but can be calculated from the smoothing data.

8.2 Auto-correlation

Suppose a user has to average several measured values of your data product. E.g., they want the mean column, 100 km around the observation site, within one month. Can you give a recommendation how they can obtain the uncertainty of this mean column, starting from the uncertainties provided for the individual columns?

Answer: Not applicable.

8.3 Correlation between main measured quantity and other quantities

Do you provide any correlation info between the main measured quantity (e.g., an ozone profile) and other quantities (e.g., a temperature profile)?

Answer: Generally not.

9. Bias handling introduced during processing

Biases can, at least in theory, be introduced during processing. For example by nonlinear measurement equations in combination with large uncertainties on the input quantities. Is this something you try to correct for, or report, or deal with in some other way? Or do you think this will be negligible?

Answer: This bias is due the error introduced by data-handling procedures such as signal averaging during varying atmospheric extinction and scattering conditions. The use of an automatic centralized procedure like the SCC can minimize this contribution and make it negligible.

10. Other remarks on data product uncertainty

Please put here any other information about the data product uncertainty that you think is important.

11. Glossary

11.1 Terms and definitions (subset used in this questionnaire)

TERM	DEFINITION	SOURCE
Bias	(1) systematic error of indication of a measuring system (2) estimate of a systematic measurement error (3) estimate of a systematic forecast error	(1) VIM/ISO:99 [RD18] (2) VIM/ISO:99 [RD18] (3) MACC [RD13]
(measurement) covariance matrix	symmetric positive semi-definite matrix of dimension N × N associated with an estimate of a real vector quantity of dimension N × 1, containing on its diagonal the squares of the standard uncertainties associated with the respective components of the estimate of the quantity, and, in its off-diagonal positions, the covariances associated with pairs of components of that estimate	GUM S2 [RD6]
Error	(1) measured quantity value minus a reference quantity value (2) difference of quantity value obtained by measurement and true value of the measurand (3) difference of forecast value and a, estimate of the true value Note: (1) and (2) refer to measurement error, while (3) refers to a forecast error	(1) VIM/ISO:99 [RD18] (2) CEOS/ISO:19159 [RD10] (3) MACC [RD13]
measurand	quantity intended to be measured	VIM/ISO:99 [RD18]
random error	(1) component of measurement error that in replicate measurements varies in an unpredictable manner; note that random measurement error equals measurement error minus systematic measurement error. Note: Random measurement errors of a set of replicate measurements form a distribution that can be summarized by its expectation, which is generally assumed to be zero, and its variance. (2) component of forecast error that varies in an unpredictable manner	(1) VIM/ISO:99 [RD18] (2) MACC [RD13]
standard uncertainty	measurement uncertainty expressed as a standard deviation	VIM/ISO:99 [RD18]

systematic error	component of measurement error that in replicate measurements remains constant or varies in a predictable manner Note that systematic measurement error, and its causes, can be known or unknown. A correction can be applied to compensate for a known systematic measurement error. (Note from GUM [RD4], 3.2.3): It is assumed that, after correction, the expectation or expected value of the error arising from a systematic effect is zero. (Note from GUM [RD4], 3.3.1): The result of a measurement after correction for recognized systematic effects is still only an estimate of the value of the measurand because of the uncertainty arising from random effects and from imperfect correction of the result for systematic effects.	VIM/ISO:99 [RD18]
uncertainty	non-negative parameter characterizing the dispersion of the quantity values being attributed to a measurand, based on the information used	VIM/ISO:99 [RD18]
standard uncertainty	measurement uncertainty expressed as a standard deviation	VIM/ISO:99 [RD18]
(1) uncertainty of measurement method, (2), (3) (community term) structural uncertainty	(1) Uncertainty associated with the method of measurement, as there can be other methods, some of them as yet unknown or in some way impractical, that would give systematically different results of apparently equal validity. (2) Uncertainty arising through the choice of approach. (3) Structural uncertainty arises because different investigators may make different plausible choices for the method (or “model”) that they apply to make corrections or “adjustments” to the raw data.	(1) GUM [RD4], section F.2.5 (2) Thorne et al. (2005) (3) Karl (2006), p. 139

validation	(1) the process of assessing, by independent means, the quality of the data products derived from the system outputs (2) verification, where the specified requirements are adequate for an intended use (3) confirmation, through the provision of objective evidence, that the requirements for a specific intended use or application have been fulfilled (4) the process of assessing, by independent means, the degree of correspondence between the value of the radiometric quantity derived from the output signal of a calibrated radiometric device and the actual value of this quantity. (5) confirmation by examination and provision of objective evidence that specifications conform to user needs and intended uses, and that the particular requirements implemented through software can be consistently fulfilled	(1) CEOS/ISO:19159 [RD10] (2) VIM/ISO:99 [RD18] (3) ISO:9000 [RD7] (4) NIST [RD15] (5) CDRH [RD1]

11.2 Terms and definitions (full set)

TERM	DEFINITION	SOURCE
accuracy	closeness of agreement between a measured quantity value and a true quantity value of a measurand. Note that it is not a quantity and it is not given a numerical quantity value. A measurement is said to be more accurate when it offers a smaller measurement error.	VIM/ISO:99 [RD18], GUM [RD4]
area (volume) of representativeness	the area (volume) in which the concentration does not differ from the concentration at the station by more than a specific range	Larssen [RD12]
bias	(1) systematic error of indication of a measuring system (2) estimate of a systematic measurement error (3) estimate of a systematic forecast error	(1) VIM/ISO:99 [RD18] (2) VIM/ISO:99 [RD18] (3) MACC [RD13]
calibration	(1) the process of quantitatively defining the system responses to known, controlled signal inputs (2) operation that, under specified conditions, in a first step, establishes a relation between the quantity values with measurement uncertainties provided by measurement standards and corresponding indications with associated measurement uncertainties and, in a second step, uses this information to establish a relation for obtaining a measurement result from an indication	(1) CEOS/ISO:19159 [RD10] (2) VIM/ISO:99 [RD18]
climate data record (CDR)	a time series of measurements of sufficient length, consistency and continuity to determine climate variability and change	NOAA [RD16]
(measurement) covariance matrix	symmetric positive semi-definite matrix of dimension N × N associated with an estimate of a real vector quantity of dimension N × 1, containing on its diagonal the squares of the standard uncertainties associated with the respective components of the estimate of the quantity, and, in its off-diagonal positions, the covariances associated with pairs of components of that estimate	GUM S2 [RD6]

dead band (or neutral zone)	maximum interval through which a value of a quantity being measured can be changed in both directions without producing a detectable change in the corresponding indication	VIM/ISO:99 [RD18]
detection limit	measured quantity value, obtained by a given measurement procedure, for which the probability of falsely claiming the absence of a component is β, given a probability α of falsely claiming its presence	VIM/ISO:99 [RD18]
error	(1) measured quantity value minus a reference quantity value (2) difference of quantity value obtained by measurement and true value of the measurand (3) difference of forecast value and a, estimate of the true value Note: (1) and (2) refer to measurement error, while (3) refers to a forecast error	(1) VIM/ISO:99 [RD18] (2) CEOS/ISO:19159 [RD10] (3) MACC [RD13]
establish	define, document and implement	CDRH [RD1]
indication	quantity value provided by a measuring instrument or a measuring system	VIM/ISO:99 [RD18]
fiducial	used as a fixed standard of reference for comparison or measurement (fiducial point)	WordNet [RD20]
fiducial mark	index mark on a test system that allows automatic geometric identification and orientation detection of an object using imaging systems	ISO:19262 [RD11]
field-of-regard	an area of the object space scanned by the field-of-view of a scanning sensor	NIST [RD15]
field-of-view	the solid angle from which the detector receives radiation	NIST [RD15]
footprint	the area of a target encircled by the field-of-view of a detector of radiation, or irradiated by an active system	NIST [RD15]
geometrical resolution	ability of a sensor system to record signals separately from neighboring object structures	DIN 18716-3 [RD3]
ground sampling distance (GSD)	linear distance between pixel centres on the ground	CEOS/ISO:19159 [RD10]
influence quantity	quantity that, in a direct measurement, does not affect the quantity that is actually measured, but affects the relation between the indication and the measurement result	VIM/ISO:99 [RD18]
in situ measurement	(1) a direct measurement of the measurand in its original place (2) any sub-orbital measurement of the measurand	(1) CEOS/ISO:19159 [RD10] (2) GEOSS

instantaneous field of view (IFOV)	opening angle corresponding to one detector element	ISO:19130 [RD9]
instrumental drift	continuous or incremental change over time in indication, due to changes in metrological properties of a measuring instrument. Note that instrumental drift is related neither to a change in a quantity being measured nor to a change of any recognized influence quantity.	VIM/ISO:99 [RD18]
measurand	quantity intended to be measured	VIM/ISO:99 [RD18]
metadata	data about the data; parameters that describe, characterise, and/or index the data	WMO [RD19]
monitoring	(1) systematic evaluation over time of some quantity (2) by extension, evaluation over time of the performance of a system, of the occurrence of an event etc.	(1) NIST [RD15] (2) MACC [RD13]
point-to-area (point-to-volume) representativeness	the probability that a point measurement lies within a specific range of area-average (volume-average) concentration value	Nappo [RD14]
positional accuracy	closeness of coordinate value to the true or accepted value in a specified reference system	ISO:19116 [RD8]
precision	(1) measure of the repeatability of a set of measurements. Note that precision is usually expressed as a statistical value based upon a set of repeated measurements such as the standard deviation from the sample mean (2) closeness of agreement between indications or measured quantity values obtained by replicate measurements on the same or similar objects under specified conditions	(1) ISO:19116 [RD8] (2) VIM/ISO:99 [RD18]
procedure	specified way to carry out an activity or a process	ISO:9000 [RD7]
process	set of interrelated or interacting activities that use inputs to deliver an intended result	ISO:9000 [RD7]
process validation	establishing documented evidence of a high degree of assurance that a specific process will consistently produce a product meeting its pre-determined specifications and quality characteristics	CDRH [RD1]
product	output of an organization that can be produced without any transaction taking place between the organization and the customer	ISO:9000 [RD7]
quality	degree to which a set of inherent characteristics of an object fulfils requirements	ISO:9000 [RD7]

quality assurance	part of quality management focused on providing confidence that quality requirements will be fulfilled	CEOS/ISO:19159 [RD10], ISO:9000 [RD7]
quality assessment	term referring to the derivation of quality indicators providing sufficient information to assess whether quality requirements are fulfilled	CEOS
quality control (QC)	(1) QC refers to the activities undertaken to check and optimise accuracy and precision of the data after its collection (2) part of quality management focused on fulfilling quality requirements	(1) CEOS/ISO:19159 [RD10] (2) ISO:9000 [RD7]
quality indicator (QI)	a means of providing a user of data or derived product with sufficient information to assess its suitability for a particular application. This information should be based on a quantitative assessment of its traceability to an agreed reference or measurement standard (ideally SI), but can be presented as a numeric or a text descriptor, provided the quantitative linkage is defined.	QA4EO [RD17]
radiometric calibration	a determination of radiometric instrument performance in the spatial, spectral, and temporal domains in a series of measurements, in which its output is related to the true value of the measured radiometric quantity	NIST [RD15]
random error	(1) component of measurement error that in replicate measurements varies in an unpredictable manner; note that random measurement error equals measurement error minus systematic measurement error. Note: Random measurement errors of a set of replicate measurements form a distribution that can be summarized by its expectation, which is generally assumed to be zero, and its variance. (2) component of forecast error that varies in an unpredictable manner	(1) VIM/ISO:99 [RD18] (2) MACC [RD13]
relative standard uncertainty	standard measurement uncertainty divided by the absolute value of the measured quantity value	VIM/ISO:99 [RD18]
repeatability	measurement precision under set of conditions including the same measurement procedure, same operator, same measuring system, same operating conditions and same location, and replicated measurements over a short period of time	VIM/ISO:99 [RD18]

representativeness	the extent to which a set of measurements taken in a given space-time domain reflect the actual conditions in the same or different space-time domain taken on a scale appropriate for a specific application	Nappo [RD14]
reproducibility	measurement precision under a set of conditions including different locations, operators, and measuring systems	VIM/ISO:99 [RD18]
resolution	(1) smallest change in a quantity being measured that causes a perceptible change in the corresponding indication (2) the least angular/linear/temporal/spectral distance between two identical point sources of radiation that can be distinguished according to a given criterion (3) the least vertical/geographical/temporal distance between two identical atmospheric features that can be distinguished in a gridded numerical product or in time series of measurements; resolution is equal to or coarser than vertical/geographical/temporal sampling of the grid or the measurement time series	(1) VIM/ISO:99 [RD18] (2) NIST [RD15] (3) MACC [RD13]
service	output of an organization with at least one activity necessarily performed between the organization and the customer	ISO:9000 [RD7]
stability	Property of a measuring instrument, whereby its metrological properties remain constant in time	VIM/ISO:99 [RD18]
standard uncertainty	measurement uncertainty expressed as a standard deviation	VIM/ISO:99 [RD18]
systematic error	component of measurement error that in replicate measurements remains constant or varies in a predictable manner Note that systematic measurement error, and its causes, can be known or unknown. A correction can be applied to compensate for a known systematic measurement error. (Note from GUM [RD4], 3.2.3): It is assumed that, after correction, the expectation or expected value of the error arising from a systematic effect is zero. (Note from GUM [RD4], 3.3.1): The result of a measurement after correction for recognized systematic effects is still only an estimate of the value of the measurand because of the uncertainty arising from random effects and from imperfect correction of the result for systematic effects.	VIM/ISO:99 [RD18]
system	set of interrelated or interacting elements	ISO:9000 [RD7]

traceability	(1) (*metrological traceability*) property of a measurement result relating the result to a stated metrological reference (free definition and not necessarily SI) through an unbroken chain of calibrations of a measuring system or comparisons, each contributing to the stated measurement uncertainty (2) ability to trace the history, application or location of an object, a product or a service	(1) VIM/ISO:99 [RD18] (2) ISO:9000 [RD7]
traceability chain	sequence of measurement standards and calibrations that is used to relate a measurement result to a reference	VIM/ISO:99 [RD18]
uncertainty	non-negative parameter characterizing the dispersion of the quantity values being attributed to a measurand, based on the information used	VIM/ISO:99 [RD18]
(1) uncertainty of measurement method, (2), (3) (community term) structural uncertainty	(1) Uncertainty associated with the method of measurement, as there can be other methods, some of them as yet unknown or in some way impractical, that would give systematically different results of apparently equal validity. (2) Uncertainty arising through the choice of approach. (3) Structural uncertainty arises because different investigators may make different plausible choices for the method (or “model”) that they apply to make corrections or “adjustments” to the raw data.	(1) GUM [RD4], section F.2.5 (2) Thorne et al. (2005) (3) Karl (2006), p. 139
validation	(1) the process of assessing, by independent means, the quality of the data products derived from the system outputs (2) verification, where the specified requirements are adequate for an intended use (3) confirmation, through the provision of objective evidence, that the requirements for a specific intended use or application have been fulfilled (4) the process of assessing, by independent means, the degree of correspondence between the value of the radiometric quantity derived from the output signal of a calibrated radiometric device and the actual value of this quantity. (5) confirmation by examination and provision of objective evidence that specifications conform to user needs and intended uses, and that the particular requirements implemented through software can be consistently fulfilled	(1) CEOS/ISO:19159 [RD10] (2) VIM/ISO:99 [RD18] (3) ISO:9000 [RD7] (4) NIST [RD15] (5) CDRH [RD1]

verification	(1) provision of objective evidence that a given item fulfils specified requirements; note that, when applicable, measurement uncertainty should be taken into consideration. (2) confirmation, through the provision of objective evidence, that specified requirements have been fulfilled (3) the provision of objective evidence that the design outputs of a particular phase of the software development life cycle meet all of the specified requirements for that phase	(1) VIM/ISO:99 [RD18] (2) ISO:9000 [RD7] (3) CDRH [RD1]
vicarious calibration	post-launch calibration of sensors that make use of natural or artificial sites on the surface of the Earth	CEOS/ISO:19159 [RD10]

11.3 References for terms and definitions

11.3.1 International standards and frameworks

[RD1] CDRH
Center for Devices and Radiological Health (CDRH), General Principles of Software Validation; Final Guidance for Industry and FDA Staff, CBER CDRH/OC Doc. N. 938, January 11, 2002. Publicly available via http://www.fda.gov/RegulatoryInformation/Guidances/ucm085281.htm

[RD2] CEOS
CEOS Committee on Earth Observation Satellites (CEOS): Terms and Definitions and other documents and resources publicly available on http://calvalportal.ceos.org.

[RD3] DIN 18716-3
DIN 18716-3: 1997-07, Photogrammetry and remote sensing - Part 3: Remote sensing terms

[RD4] GUM
Joint Committee for Guides in Metrology (JCGM/WG 1) 100:2008, Evaluation of measurement data – Guide to the expression of uncertainty in a measurement (GUM), ISO/IEC Guide 98-3:2008,
http://www.bipm.org/utils/common/documents/jcgm/JCGM_100_2008_E.pdf

[RD5] GUM S1
Joint Committee for Guides in Metrology (JCGM/WG 1) 101:2008, Evaluation of measurement data - Supplement 1 to the "Guide to the expression of uncertainty in measurement" - Propagation of distributions using a Monte Carlo method, ISO/IEC Guide 98-3/Suppl.1:2008,
http://www.bipm.org/utils/common/documents/jcgm/JCGM_101_2008_E.pdf

[RD6] GUM S2
Joint Committee for Guides in Metrology (JCGM/WG 1) 102:2011, Evaluation of measurement data - Supplement 2 to the "Guide to the expression of uncertainty in measurement" - Extension to any number of output quantities, ISO/IEC Guide 98-3:2008/Suppl.2:2011,
http://www.bipm.org/utils/common/documents/jcgm/JCGM_102_2011_E.pdf

[RD7] ISO:9000
ISO 9000:2015(en), Quality management systems - Fundamentals and vocabulary

[RD8] ISO:19116
ISO 19116:2004(en), Geographic information - Positioning services

[RD9] ISO:19130
ISO/TS 19130-2:2014(en), Geographic information - Imagery sensor models for geopositioning - Part 2: SAR, InSAR, lidar and sonar

[RD10] ISO:19159
ISO/TS 19159-1:2014(en), Geographic information - Calibration and validation of remote sensing imagery sensors and data — Part 1: Optical sensors

[RD11] ISO:19262
ISO:19262:2015(en), Photography — Archiving Systems — Vocabulary

[RD12] Larrsen
Larssen, S., R. Sluyter, and C. Helmis, Criteria for EUROAIRNET – The EEA Air Quality Monitoring and Information Network, 1999.

[RD13] MACC
MACC II Service Validation Protocol, Deliverable D153.1, May 2013, http://www.gmes-atmosphere.eu/documents/maccii/deliverables/man/MACCII_MAN_DEL_D_153.1_20130528_Lambert_V2.pdf

[RD14] Nappo
Nappo, C.J., Caneill J.Y., Furman R.W., Gifford F.A., Kaimal J.C., Kramer M.L., Lockhart T.J., Pendergast M.M, Pielke R.A., Randerson D., Shreffler J.H., and Wyngaard J.C., The Workshop on the Representativeness of Meteorological Observations, June 1981, Boulder, CO, Bull. Am. Meteorol. Soc. 63, 761-764, 1982.

[RD15] NIST
Prokhorov, A. V., R. U. Datla, V. P. Zakharenkov, V. Privalsky, T. W. Humpherys, and V. I. Sapritsky, Spaceborne Optoelectronic Sensors and their Radiometric Calibration. Terms and Definitions. Part 1. Calibration Techniques, Ed. by A. C. Parr and L. K. Issaev, NIST Technical Note NISTIR 7203, March 2005

[RD16] NOAA
Climate Data Records from Environmental Satellites: Interim Report, Committee on Climate Data Records from NOAA Operational Satellites; Board on Atmospheric Sciences and Climate; Division on Earth and Life Studies; National Research Council (2004), DOI: 10.17226/10944

[RD17] QA4EO
QA4EO – A Quality Assurance framework for Earth Observation, established by the CEOS. It consists of ten distinct key guidelines linked through an overarching document (the QA4EO Principles) and more community-specific QA4EO procedures, all available on http://qa4eo.org/documentation.html A short QA4EO "user" guide has been produced to provide background into QA4EO and how one would start implementing it (http://qa4eo.org/docs/QA4EO_guide.pdf)

[RD18] VIM/ISO:99
Joint Committee for Guides in Metrology (JCGM/WG 2) 200:2012 & ISO/IEC Guide 99-12:2007, International Vocabulary of Metrology – Basic and General Concepts and Associated Terms (VIM), http://www.bipm.org/en/publications/guides/vim.html

[RD19] WMO

WMO Quality Management Framework (QMF), home page at http://www.bom.gov.au/wmo/quality_management.shtmll

[RD20] WordNet
Princeton University "About WordNet." WordNet. Princeton University. 2010, http://wordnet.princeton.edu.

11.3.2 Other references

Deeter, M. N., S. Martinez-Alonso, D. P. Edwards, L. K. Emmons, J. C. Gille, H. M. Worden, J. V. Pittman, B. C. Daube, and S. C. Wofsy. 2013. Validation of MOPITT Version 5 thermal-infrared, near-infrared, and multispectral carbon monoxide profile retrievals for 2000-2011. J. Geophys. Res. 118:6710–6725.

Karl, T. R. (Ed.). 2006. Temperature Trends in the Lower Atmosphere. Steps for Understanding and Reconciling Differences.

Thorne, P. W., D. E. Parker, J. R. Christy, and C. A. Mears. 2005. Uncertainties in climate trends: lessons from upper-air temperature records. Bull. Am. Meteorol. Soc. 86:1437–1442.

Annex B

GAIA-CLIM questionnaire about uncertainty in data products

Lidar – Water vapour profiles

Table of Contents

1. Identification of respondent and of data product

What are your contact details?

Answer:

Arnoud Apituley
KNMI - Royal Netherlands Meteorological Institute
P.O. Box 201, 3730 AE De Bilt
Ph: +31 6 55457540
apituley@knmi.nl

For which data product are you filling in this questionnaire?

Answer: Raman lidar measurements of water vapour vertical profiles of mixing ratio

Please provide one or more accessible sources of information that a non-expert user can refer to, to gain an understanding of the measurement technique.

Answer:

Wandinger, U., 2005: Introduction to lidar. Lidar: Range-Resolved Optical Remote Sensing of the Atmosphere, C. Weitkamp, Ed., Springer Series of Optical Sciences, Vol. 102, Springer, 1–18.

Wandinger, U., 2005: Introduction to lidar. Lidar: Range-Resolved Optical Remote Sensing of the Atmosphere, C. Weitkamp, Ed., Springer Series of Optical Sciences, Vol. 102, Springer, pp. 256–261.

2. Recommended literature

Which literature work would you recommend to understand better the measurement technique and the ***general uncertainty framework*** *within which uncertainties of the data product are constructed. Note that for metrology, the vocabulary list of the VIM (*International Vocabulary of Metrology*), and the uncertainty framework of the GUM (Guide to expression of uncertainty,) are important standards. Please provide a complete reference or doi where possible.*

Answer:

Wandinger, U., 2005: Introduction to lidar. Lidar: Range-Resolved Optical Remote Sensing of the Atmosphere, C. Weitkamp, Ed., Springer Series of Optical Sciences, Vol. 102, Springer, 1–18.

More specifically, which literature works (article, ATBD, other…) would you recommend to understand better how uncertainties of ***this particular data product*** *are conceived? Please provide a complete reference or doi where possible.*

Answer:

Leblanc, T., McDermid, I. S., and Walsh, T. D.: Ground-based water vapor raman lidar measurements up to the upper troposphere and lower stratosphere for long-term monitoring, Atmos. Meas. Tech., 5, 17-36, doi:10.5194/amt-5-17-2012, 2012.

Whiteman, D. N., Cadirola, M., Venable, D., Calhoun, M., Miloshevich, L., Vermeesch, K., Twigg, L., Dirisu, A., Hurst, D., Hall, E., Jordan, A., and Vömel, H.: Correction technique for Raman water vapor lidar signal-dependent bias and suitability for water vapor trend monitoring in the upper troposphere, Atmos. Meas. Tech., 5, 2893-2916, doi:10.5194/amt-5-2893-2012, 2012.

Please specify also if the literature source is still up-to-date with the current data product. If not, where can a user find the information on the latest version of the data product and its uncertainties?

Answer:

3. Main measured quantity (measurand)

3.1 Specification of measurand

Specify the main measured quantities (i.e., the measurands) and the associated unit of the data product, along with their field name in the data product

Example measurands with unit: Temperature [K], O3 profile [ppmv], water vapour [ppmv]

Quantity [unit]	Field name
Water vapour [g/kg]	Water_vapor_mixing_ratio

3.2 Measurement equation

What is the relation between the main measured quantity of the data product and input quantities? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to literature publications).

Answer:

The lidar equation is relates the light power backscattered by the atmospheric target with the signal collected by the lidar receiver. In a general form, lidar equation can be written as

$$P(\lambda_L,\lambda_S,z)=P_L(\lambda_L)\Psi(\lambda_S,\lambda_L)O(z)\beta(\lambda_S,\lambda_L,\theta,z)\frac{A}{z^2}\frac{c\tau_d}{2}\exp\left(-\int_0^z\alpha(z)dz\right)+P_B \qquad \text{[Eq.1]}$$

where:

$P(\lambda_L,\lambda_S,z)$ is the backscattered power received from the distance z from the source (zenith pointing), at a specific wavelength λ_s, due to the scattering of the laser wavelength λ_L;

$\Psi(\lambda_S,\lambda_L)=\xi(\lambda_L,\lambda_S)\eta(\lambda_S)$ is transmission of the lidar receiver, given by $\xi(\lambda_L,\lambda_S)$ that is the optical efficiency of the lidar receiver, including such factors as the reflectivity of the telescope and the transmission of the conditioning optics, while $\eta(\lambda_S)$ is the quantum efficiency of the receiver and detection parts;

$O(z)$ is the system overlap function;

$P_L(\lambda_L)$ is the output laser power at the wavelength λ_L;
$\beta(\lambda_S, \lambda_L, \theta, z)$ is the volume scattering coefficient at the distance z and at an angle θ and represents the probability that a transmitted photon is backscattered by the atmosphere into a unit solid angle ($\theta = \pi$);
$\frac{A}{z^2}$ is the probability that a scatter photon from the distance is collected by the receiving telescope of surface A;
$\frac{c\tau_d}{2}$ represents the sounding vertical resolution, where c and τ_d are respectively the light speed and the dwell time (i.e. the laser duration pulse);
$\exp\left(-\int_0^z \alpha(z)dz\right)$ is the two-way transmissivity of the light from laser source to the distance z and from distance z to the receiver, respectively;
P_B is the contribution power return due to the background light.

To use of [Eq.1] for the inversion of the backscattered radiation and to retrieve the atmospheric parameters, the approximation of single scattering is used: this means that a photon is scattered only once by the atmospheric constituents and that these are separated adequately and are moving randomly. Thus, multiple scattering events are neglected and the contribution to the total scattered energy by many targets have no phase relation and the total intensity is simply the sum of the intensity scattered from each target.

For water vapour, use is made of two inelastically scattered signals. In [Eq.1] we replace λ_s by λ_{H_2O} (i.e. Raman shifted wavelength by water vapour) and λ_{N_2} (Raman shifted wavelength by nitrogen), and take the ratio of these two signals:

$$R(z) = \frac{P(\lambda_L, \lambda_{H_2O}, z)}{P(\lambda_L, \lambda_{N_2}, z)} = \kappa_{eff}\kappa_O\kappa_\sigma\kappa_\alpha\frac{N_{H_2O}(z)}{N_{N_2}(z)}$$

[Eq.2]

κ_{eff} is a constant expressing the ratio of all the optical and quantum efficiencies of the receivers as well as other constant terms, $\kappa_{\text{O}}(r)$ is the ratio of the overlap functions of the nitrogen and water vapour channels, $\kappa_\sigma(r)$ is the ratio of the nitrogen and water vapour Raman cross-sections, and $\kappa_\alpha(r)$ is the ratio of the particulate extinction along the return path of the beam at the nitrogen and water vapour wavelengths (often referred to as "extinction differential").
After calibration, if follows that the water vapour mixing ratio *q(r)* is:

$$q(z) = \kappa_{eff}(z)\kappa_O(z)\kappa_\sigma(z)\kappa_\alpha(z)R(z)$$

[Eq.3]

4. Traceability and comparability

4.1 SI or community traceability

Is the measurement quantity traceable, via an unbroken chain of processing steps, to SI units or community accepted standards?

Answer: Yes. However, different calibration methods can be applied, leading to different traceability chains.

If yes, please provide references to available literature describing the traceability aspects of the measurement.

Leblanc, T., McDermid, I. S., and Walsh, T. D.: Ground-based water vapor raman lidar measurements up to the upper troposphere and lower stratosphere for long-term monitoring, Atmos. Meas. Tech., 5, 17-36, doi:10.5194/amt-5-17-2012, 2012.

If no, please describe what aspects of the measurement are not fully traceable and how this aspect is addressed in deriving the data product and its uncertainty.

4.2 Comparability

If measurements are taken at multiple sites, are efforts made to ensure sufficiently similar measurement technique approaches to ensure comparability? Please provide links to any supporting materials available such as instrument manuals / network protocols.

Answer: Yes.

- Intercomparison campaigns have been carried out in the framework of NDACC:

Measurements of Humidity in the Atmosphere and Validation Experiments (MOHAVE)-2009: overview of campaign operations and results
T. Leblanc, T. D. Walsh, I. S. McDermid, G. C. Toon, J.-F. Blavier, B. Haines, W. G. Read, B. Herman, E. Fetzer, S. Sander, T. Pongetti, D. N. Whiteman, T. G. McGee, L. Twigg, G. Sumnicht, D. Venable, M. Calhoun, A. Dirisu, D. Hurst, A. Jordan, E. Hall, L. Miloshevich, H. Vömel, C. Straub, N. Kampfer, G. E. Nedoluha, R. M. Gomez, K. Holub, S. Gutman, J. Braun, T. Vanhove, G. Stiller, and A. Hauchecorne, Atmos. Meas. Tech., 4, 2579-2605, doi:10.5194/amt-4-2579-2011, 2011

Correction technique for Raman water vapor lidar signal-dependent bias and suitability for water vapor trend monitoring in the upper troposphere
D. N. Whiteman, M. Cadirola, D. Venable, M. Calhoun, L. Miloshevich, K. Vermeesch, L. Twigg, A. Dirisu, D. Hurst, E. Hall, A. Jordan, and H. Vömel, Atmos. Meas. Tech., 5, 2893-2916, doi:10.5194/amt-5-2893-2012, 2012

Ground-based water vapor raman lidar measurements up to the upper troposphere and lower stratosphere for long-term monitoring

T. Leblanc, I. S. McDermid, and T. D. Walsh, Atmos. Meas. Tech., 5, 17-36, doi:10.5194/amt-5-17-2012, 2012

- In 2008 a campaign was conducted using and airborne water vapour differential absorption lidar, that overpassed several ground based water vapour Raman lidar systems:

Trickl, T., Vogelmann, H., Fix, A., Schäfler, A., Wirth, M., Calpini, B., Levrat, G., Romanens, G., Apituley, A., Wilson, K. M., Begbie, R., Reichardt, J., Vömel, H., and Sprenger, M.: How stratospheric are deep stratospheric intrusions? LUAMI 2008, Atmos. Chem. Phys., 16, 8791-8815, doi:10.5194/acp-16-8791-2016, 2016.

- Furthermore, Raman systematic lidar validation has been done in other stations:

Brocard, E., Philipona, R., Haefele, A., Romanens, G., Mueller, A., Ruffieux, D., Simeonov, V., and Calpini, B.: Raman Lidar for Meteorological Observations, RALMO – Part 2: Validation of water vapor measurements, Atmos. Meas. Tech., 6, 1347-1358, doi:10.5194/amt-6-1347-2013, 2013.

Jens Reichardt, Ulla Wandinger, Volker Klein, Ina Mattis, Bernhard Hilber, and Robert Begbie, "RAMSES: German Meteorological Service autonomous Raman lidar for water vapor, temperature, aerosol, and cloud measurements," Appl. Opt. 51, 8111-8131 (2012)

A. Apituley, K.M. Wilson, C. Potma, H. Volten, and M. de Graaf. Performance assessment and application of Caeli – a high-performance Raman lidar for diurnal profiling of water vapour, aerosols and clouds. In A. Apituley, H.W.J. Russchenberg, and W.A.A. Monna, editors, *Proceedings of the 8th ISTP*, pages S06–O10, 2009.

- In the US experiments have been carried out aimed at the dynamics of water vapour:

Turner, D., R. Ferrare, V. Wulfmeyer, and A. Scarino, 2014: Aircraft Evaluation of Ground-Based Raman Lidar Water Vapor Turbulence Profiles in Convective Mixed Layers. J. Atmos. Oceanic Technol., 31, 1078–1088, doi: 10.1175/JTECH-D-13-00075.1.

5. Representation of the uncertainty in the data product

5.1 Uncertainty field name(s)

Which field name(s) are used in the data product to hold the uncertainty value(s) associated with the main measured quantities? Note that more than one uncertainty field name can be associated with a single quantity (e.g., one field name for the "uncertainty due to random effects" and one for the "uncertainty due to systematic effects").

Field name of uncertainty	Associated quantity
Error	Random uncertainty

5.2 Uncertainty form

In what form is the uncertainty per measurement represented in the data product? For example, is it:

- *A standard uncertainty (i.e., uncertainty expressed as standard deviation)*
- *A 95% coverage interval*
- *A variance-covariance matrix (if so, explain between which quantities the covariance is taken into account)*
- *A probability density function*
- *Other [please specify]*

Answer:
Standard uncertainty (i.e., uncertainty expressed as standard deviation) with respect to the random error in the lidar signals. Uncertainties related to the calibration method used are also included.

6. Uncertainty calculation

6.1 Formula/procedure

What is the formula/procedure by which the uncertainty is calculated? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to one or more equations in the literature).

Answer:
The procedures are described in:

Leblanc, T., McDermid, I. S., and Walsh, T. D.: Ground-based water vapor raman lidar measurements up to the upper troposphere and lower stratosphere for long-term monitoring, Atmos. Meas. Tech., 5, 17-36, doi:10.5194/amt-5-17-2012, 2012.

Is the uncertainty obtained by:

- *Uncertainty propagation, taking into account the uncertainties of the input quantities,*
- *Probability density function propagation,*
- *Sensitivity analysis: i.e., varying parameters and check the impact on the output quantity,*
- *Or still some other procedure?*

Answer:
There are two main approaches: One approach consists of calculating every single term of Eq. (3) linking R(z) and q(z). Since this task is complex and has many sources of uncertainty (including – but not limited to – the accuracy of the lidar parts' manufacturer specifications and the determination of the Raman water vapour cross-section), the resulting calibration overall accuracy using this approach is rarely found to be better than 10 %.
A second approach consists of estimating and/or minimizing any height-dependent term in Eq. (3) (namely, the ratio of the overlap functions, differential aerosol extinction, and temperature dependence of the ratio of the Raman water vapour and nitrogen cross-sections), and reduce all the terms of this equation to a single, height-independent proportionality constant. This constant can then be deduced by scaling the lidar ratios to one (or a set of) well-known water vapour

mixing ratio value(s) measured by another technique. Radiosonde measurement in the troposphere is the most common source used today. Another common source of calibration is the Total Precipitable Water (TPW) measurement from a co-located GPS or microwave radiometer. When using an external measurement, the accuracy of the calibration procedure follows that of the measurement used.

6.2 Level of approximation

In what way is the uncertainty calculation procedure an approximation?

- *Is it based on (as is common practice) a first-order Taylor approximation (see GUM, Eq. (13))*

$$u_c^2(y) = \sum_{i=1}^{N}\sum_{j=1}^{N} \frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j} u(x_i, x_j) = \sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N} \frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j} u(x_i, x_j)$$

  which will not be exact if f is nonlinear.
- *Are correlations between input quantities neglected?*
- *Other approximations?*

Answer:
Correlations between input quantities are neglected. Different error sources of the algorithm are assumed independent and uncorrelated, which is not strictly valid though might be considered negligible in a first approximation. This is the case gluing of two lidar signal measured at the same wavelength but using different detection modes, for example. For the vertical smoothing of the aerosol profiles, which is mandatory for the retrieval of the water vapour profiles, a low pass filter is typically applied acting on the final product or alternatively on the raw input signal. In this case, an effective resolution profile is provided along with the aerosol extinction and backscatter profiles which is the results of the correlation between the smoothed points. The error propagation is described in:

Leblanc, T., Sica, R. J., van Gijsel, J. A. E., Godin-Beekmann, S., Haefele, A., Trickl, T., Payen, G., and Gabarrot, F.: Proposed standardized definitions for vertical resolution and uncertainty in the NDACC lidar ozone and temperature algorithms – Part 1: Vertical resolution, Atmos. Meas. Tech., 9, 4029-4049, doi:10.5194/amt-9-4029-2016, 2016.

If an approximation is involved, do you think the approximation can be a problem, or do you consider it justified?

Answer:
The approximation becomes problematic if uncertainties are under or overestimated since the ability to use the time series for trend analysis is affected. See e.g.

Boers, R., and E. van Meijgaard (2009), What are the demands on an observational program to detect trends in upper tropospheric water vapor anticipated in the 21st century? Geophys. Res. Lett., 36, L19806, doi:10.1029/2009GL040044.

The present study indicates that for a program of upper level specific humidity observations at a midlatitude site of Cabauw, at least 50 years of radiosonde ascents will be necessary with a sampling rate of every four days using a measurement device with an accuracy of 10% or better to demonstrate that a statistically significant trend is present. This is a daunting requirement for an observation program and arguments in favor of such a program would need to be weighted against diverging scientific or economic considerations. Such considerations include those favoring systems that can sample with much higher frequency but may not always have comparable accuracies (for example a Raman – lidar system).

Although many remote sensing systems may not have the same accuracy as in situ systems in measuring climatically important variables, they do have the advantage of being able to sample atmospheric regions that are inaccessible by other means with unsurpassed sampling rates. A high sampling frequency is a powerful means of reducing the uncertainty of a mean observation. In statistical terms: The uncertainty of the mean is inversely proportional to the square root of the number of observations. So, if one observation system can sample the same parameter 100 times as frequent as another system, then we can accept a measurement uncertainty of the former that is 10 times as large as that of the latter system.

7. Uncertainty contributions

7.1 Prior

Is there a prior contribution? If so, is this prior based on measured data, a model, a rough guess, or something else?

Answer:
Scattering from molecules used as a lidar calibration source can be calculated from air pressure and temperature profiles taken from radiosonde launches, from atmospheric models (e.g. US standard atmosphere), or analysis data sets of numerical weather prediction models.
For the calibration, external sources are used. Typically radiosondes, GNSS, or microwave radiometers.

7.2 Smoothing error

Is an error source "smoothing error" included in the uncertainty calculation? If so, what do you define as "smoothing error"? Should the averaging kernel of the data product be applied in some way, before the uncertainty can be properly interpreted?

Answer:
Smoothing errors and the effect on resolution and uncertainty are extensively described in:

Leblanc, T., Sica, R. J., van Gijsel, J. A. E., Godin-Beekmann, S., Haefele, A., Trickl, T., Payen, G., and Gabarrot, F.: Proposed standardized definitions for vertical resolution and uncertainty in the NDACC lidar ozone and temperature algorithms – Part 1: Vertical resolution, Atmos. Meas. Tech., 9, 4029-4049, doi:10.5194/amt-9-4029-2016, 2016.

7.3 Noise

Is there a noise contribution? If so, what do you define as "noise"? (E.g., for MOPITT, one considers an instrumental noise, but also a "geophysical noise" (Deeter, 2013).)

Answer:
Yes, this is due to the background noise measured on each single or integrated lidar signal before the processing, subtracted in according to the solution of the lidar equation (see term P_B in Eq.1). In addition, the noise due to dark currents (instrumental noise due to the electronics), which provides a sort bias on the collected signal in analog detection mode, is measured before or after each measurement session by obscuring the instrument receiver and is then subtracted from the signals during the signal processing.

7.4 Random and systematic contributions

Do you consider explicitly separately "random", "structured random" and "systematic" contributions? If so, how do you define each of these in your calculation?

Answer:
Main sources of uncertainties for the water vapour concentration are:

- the random error that is due to signal detection,
- the systematic error associated with the estimate of temperature and pressure profiles,
- the systematic error associated with the estimate of aerosol extinction profiles,
- the error introduced by data-handling procedures such as signal averaging during varying atmospheric extinction and scattering conditions.
- largest extinction uncertainties are caused by the overlap function O(z) [Wandinger and Ansmann, 2002].
- calibration error.

7.5 Input quantities / other parameters

If the main measured quantities of the data product depend on input quantities, how do the final uncertainties depend on uncertainties of these input quantities? Please provide a list with input quantities of which the uncertainties:

1. *Are taken into account.*
2. *Could be important, but are not taken into account. For example, because their consideration would be technically difficult, or it is not clear how to estimate the associated uncertainty.*
3. *Are not taken into account, as they can be demonstrated to be negligible.*

If this list is already available somewhere in a literature source, you can simply refer to it.

Input quantity/other parameter	associated uncertainty or "important but ignored" or "negligible"	Extra info (e.g., random, systematic)
Lidar ratio	Important (decreases with the wavelength)	systematic
Calibration backscattering value	Important (increases with the wavelength)	systematic
Angstrom coefficient	negligible	systematic
Error associated with the estimate of temperature and pressure profiles	negligible	systematic

7.6 Uncertainty due to model error

Do you consider explicitly an uncertainty contribution due to the fact that the model is not perfect? Such uncertainty can be revealed e.g., by comparing results of several retrieval models.

Answer:
See above the description at section 7.4 of the error associated with the estimate of temperature and pressure profiles.

8. Correlations/covariances

8.1 Presence in data product

Do you provide correlations or covariances within your data product, directly relevant to the main measured quantity? If so, between which quantities?

Answer:
No. As mentioned above each profile is accompanied by a profiles indicating the effective vertical resolution which is the result of the applied smoothing filtering. The related covariance matrix is not provided but can be calculated from the smoothing data.

Please state in the table below which of the quantities are reported and/or included in the total error. Please use either yes, no or N/A for the first 2 columns and a short explanation in the 3rd. column. Add other quantities as relevant.

8.2 Auto-correlation

Suppose a user has to average several measured values of your data product. E.g., they want the mean column, 100 km around the observation site, within one month. Can you give a recommendation how they can obtain the uncertainty of this mean column, starting from the uncertainties provided for the individual columns?

Answer: N/A

8.3 Correlation between main measured quantity and other quantities

Do you provide any correlation info between the main measured quantity (e.g., an ozone profile) and other quantities (e.g., a temperature profile)?

Answer:
In general not. However, there are interdependencies of the water vapour profile with the temperature profile, as well as the presence of aerosol. These effects are described the following papers.

David N. Whiteman, "Examination of the traditional Raman lidar technique. I. Evaluating the temperature-dependent lidar equations," Appl. Opt. 42, 2571-2592 (2003)

David N. Whiteman, "Examination of the traditional Raman lidar technique. II. Evaluating the ratios for water vapor and aerosols," Appl. Opt. 42, 2593-2608 (2003)

Leblanc, T., McDermid, I. S., and Walsh, T. D.: Ground-based water vapor raman lidar measurements up to the upper troposphere and lower stratosphere for long-term monitoring, Atmos. Meas. Tech., 5, 17-36, doi:10.5194/amt-5-17-2012, 2012.

9. Bias handling introduced during processing

Biases can, at least in theory, be introduced during processing. For example by nonlinear measurement equations in combination with large uncertainties on the input quantities. Is this something you try to correct for, or report, or deal with in some other way? Or do you think this will be negligible?

Answer:
This bias is due the error introduced by data-handling procedures such as signal averaging during varying atmospheric extinction and scattering conditions.

10. Other remarks on data product uncertainty

Please put here any other information about the data product uncertainty that you think is important.

Annex C

GAIA-CLIM questionnaire about uncertainty in data products

Lidar – Ozone profiles

Table of Contents

1. Identification of respondent and of data product

What are your contact details?

Answer:
Arnoud Apituley
KNMI - Royal Netherlands Meteorological Institute
P.O. Box 201, 3730 AE De Bilt
Ph: +31 6 55457540
apituley@knmi.nl

For which data product are you filling in this questionnaire?

Answer: Differential absorption lidar for ozone concentrations

Please provide one or more accessible sources of information that a non-expert user can refer to, to gain an understanding of the measurement technique.

Answer:
Wandinger, U., 2005: Introduction to lidar. Lidar: Range-Resolved Optical Remote Sensing of the Atmosphere, C. Weitkamp, Ed., Springer Series of Optical Sciences, Vol. 102, Springer, 1–18.

2. Recommended literature

*Which literature work would you recommend to understand better the measurement technique and the **general uncertainty framework** within which uncertainties of the data product are constructed. Note that for metrology, the vocabulary list of the VIM (*International Vocabulary of Metrology*), and the uncertainty framework of the GUM (Guide to expression of uncertainty) are important standards. Please provide a complete reference or doi where possible.*

Answer:
Wandinger, U., 2005: Introduction to lidar. Lidar: Range-Resolved Optical Remote Sensing of the Atmosphere, C. Weitkamp, Ed., Springer Series of Optical Sciences, Vol. 102, Springer, 1–18.

R. M. Measures. *Laser Remote Sensing*. Wiley sons, New York, 1984.

*More specifically, which literature works (article, ATBD, other…) would you recommend to understand better how uncertainties of **this particular data product** are conceived? Please provide a complete reference or doi where possible.*

Answer:

R. M. Measures. *Laser Remote Sensing*. Wiley sons, New York, 1984.

Vladimir A. Kovalev and William E. Eichinger. *Elastic Lidar: Theory, Practice, and Analysis Methods*. Wiley, 2004.

E. V. Browell, S. Ismail, and S. T. Shipley. Ultraviolet DIAL Measurements of O3 Profiles in Regions of Spatially Inhomogeneous Aerosols. *Appl. Opt.*, 24:2827–2836, 1985.

3. Main measured quantity (measurand)

3.1 Specification of measurand

Specify the main measured quantities (i.e., the measurands) and the associated unit of the data product, along with their field name in the data product

Example measurands with unit: Temperature [K], O3 profile [ppmv], water vapour [ppmv]

Quantity [unit]	Field name
ozone [molecules/m^3]	Ozone concentration

3.2 Measurement equation

What is the relation between the main measured quantity of the data product and input quantities? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to literature publications).

Answer:

The lidar equation is relates the light power backscattered by the atmospheric target with the signal collected by the lidar receiver. In a general form, lidar equation can be written as

$$P(\lambda_L,\lambda_S,z) = P_L(\lambda_L)\Psi(\lambda_S,\lambda_L)O(z)\beta(\lambda_S,\lambda_L,\theta,z)\frac{A}{z^2}\frac{c\tau_d}{2}\exp\left(-\int_0^z \alpha(z)dz\right)+P_B \qquad \text{[Eq.1]}$$

where:

$P(\lambda_L,\lambda_S,z)$ is the backscattered power received from the distance z from the source (zenith pointing), at a specific wavelength λ_s, due to the scattering of the laser wavelength λ_L;

$\Psi(\lambda_S,\lambda_L)=\xi(\lambda_L,\lambda_S)\eta(\lambda_S)$ is transmission of the lidar receiver, given by $\xi(\lambda_L,\lambda_S)$ that is the optical efficiency of the lidar receiver, including such factors as the reflectivity of the telescope and the transmission of the conditioning optics, while $\eta(\lambda_S)$ is the quantum efficiency of the receiver and detection parts;

$O(z)$ is the system overlap function;

$P_L(\lambda_L)$ is the output laser power at the wavelength λ_L;

$\beta(\lambda_S,\lambda_L,\theta,z)$ is the volume scattering coefficient at the distance z and at an angle θ and represents the probability that a transmitted photon is backscattered by the atmosphere into a unit solid angle ($\theta=\pi$);

$\frac{A}{z^2}$ is the probability that a scatter photon from the distance is collected by the receiving telescope of surface A;

$\frac{c\tau_d}{2}$ represents the sounding vertical resolution, where c and τ_d are respectively the light speed and the dwell time (i.e. the laser duration pulse);

$\exp\left(-\int_0^z \alpha(z)dz\right)$ is the two-way transmissivity of the light from laser source to the distance z and from distance z to the receiver, respectively;

P_B is the contribution power return due to the background light.

To use of [Eq.1] for the inversion of the backscattered radiation and to retrieve the atmospheric parameters, the approximation of single scattering is used: this means that a photon is scattered only once by the atmospheric constituents and that these are separated adequately and are moving randomly. Thus, multiple scattering events are neglected and the contribution to the total scattered energy by many targets have no phase relation and the total intensity is simply the sum of the intensity scattered from each target.

To apply the differential absorption lidar (DIAL) technique for ozone, use is made of two elastically scattered signals tuned to so-called on-line and off-line absorption frequencies. In [Eq.1] we replace both λ_L and λ_s by λ_{on} (i.e. an elastic lidar signal excited and detected at the on-absorption line) and a second signal is detected for the conditions where λ_L and λ_s are both replaced by λ_{off} (i.e. the off-absorption line), and take the ratio of these two signals yields in simplified form:

$$\frac{P(\lambda_{on}, z)}{P(\lambda_{off}, z)} = C\frac{\beta_{\lambda_{on}(z)}}{\beta_{\lambda_{off}(z)}} exp\left(-2\int_0^z (\sigma_{\lambda_{on}} - \sigma_{\lambda_{off}}) n_{O_3}(r)dr\right)$$

[Eq. 2]

Here $\beta_{\lambda_{on}}(z)$ and $\beta_{\lambda_{off}}(z)$ are related to aerosol and molecular scattering, while $\sigma_{\lambda_{on}}$ and $\sigma_{\lambda_{off}}$ designate the absorption cross-sections at λ_{on} and λ_{off}, respectively.

In order to retrieve the ozone concentration profile $n_{O_3}(z)$, we take the log and the derivative:

$$n_{O_3}(z) = \frac{-1}{2\Delta\sigma}\frac{d}{dz}\left(ln\frac{P(\lambda_{on}, z)}{P(\lambda_{off}, z)}\right)$$

[Eq.3]

For simplicity, we have ignored effects due to aerosols and molecular scattering, as well as interferences from other gases.

4. Traceability and comparability

4.1 SI or community traceability

Is the measurement quantity traceable, via an unbroken chain of processing steps, to SI units or community accepted standards?

Answer: Yes.

If yes, please provide references to available literature describing the traceability aspects of the measurement.

T. Leblanc, R. Sica, J. A. E. van Gijsel, S. Godin-Beekmann, A. Haefele, T. Trickl, G. Payen, and G. Liberti. Proposed standardized definitions for vertical resolution and uncertainty in the NDACC lidar ozone and temperature algorithms - Part 2: Ozone DIAL uncertainty budget. *Atmospheric Measurement Techniques Discussions*, 2016:1–55, 2016.

If no, please describe what aspects of the measurement are not fully traceable and how this aspect is addressed in deriving the data product and its uncertainty.

4.2 Comparability

If measurements are taken at multiple sites, are efforts made to ensure sufficiently similar measurement technique approaches to ensure comparability? Please provide links to any supporting materials available such as instrument manuals / network protocols.

Answer: Yes.

In NDACC, regular intercomparisons are carried out between ozone DIAL systems for stratospheric ozone, e.g.:

Steinbrecht, W., McGee, T. J., Twigg, L. W., Claude, H., Schönenborn, F., Sumnicht, G. K., and Silbert, D.: Intercomparison of stratospheric ozone and temperature profiles during the October 2005 Hohenpeißenberg Ozone Profiling Experiment (HOPE), Atmos. Meas. Tech., 2, 125-145, doi:10.5194/amt-2-125-2009, 2009.

I. Stuart McDermid, Sophie M. Godin, L. Oscar Lindqvist, T. Daniel Walsh, John Burris, James Butler, Richard Ferrare, David Whiteman, and Thomas J. McGee, "Measurement intercomparison of the JPL and GSFC stratospheric ozone lidar systems," Appl. Opt. 29, 4671-4676 (1990).

5. Representation of the uncertainty in the data product

5.1 Uncertainty field name(s)

Which field name(s) are used in the data product to hold the uncertainty value(s) associated with the main measured quantities? Note that more than one uncertainty field name can be associated *with a single quantity (e.g., one field name for the "uncertainty due to random effects" and one for the "uncertainty due to systematic effects").*

Field name of uncertainty	Associated quantity
Error	Random uncertainty

5.2 Uncertainty form

In what form is the uncertainty per measurement represented in the data product? For example, is it:

- *A standard uncertainty (i.e., uncertainty expressed as standard deviation)*
- *A 95% coverage interval*
- *A variance-covariance matrix (if so, explain between which quantities the covariance is taken into account)*
- *A probability density function*
- *Other [please specify]*

Answer:
Standard uncertainty (i.e., uncertainty expressed as standard deviation) with respect to the random error in the lidar signals.

6. Uncertainty calculation

6.1 Formula/procedure

What is the formula/procedure by which the uncertainty is calculated? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to one or more equations in the literature).

Answer:
The background and procedures are described in:

T. Leblanc, R. Sica, J. A. E. van Gijsel, S. Godin-Beekmann, A. Haefele, T. Trickl, G. Payen, and G. Liberti. Proposed standardized definitions for vertical resolution and uncertainty in the NDACC lidar ozone and temperature algorithms - Part 2: Ozone DIAL uncertainty budget. *Atmospheric Measurement Techniques Discussions*, 2016:1–55, 2016.

Is the uncertainty obtained by:

- *Uncertainty propagation, taking into account the uncertainties of the input quantities,*
- *Probability density function propagation,*
- *Sensitivity analysis: i.e., varying parameters and check the impact on the output quantity,*
- *Or still some other procedure?*

Answer:
A standardized approach for the definition, propagation, and reporting of uncertainty in the ozone differential absorption lidar data products contributing to the Network for the Detection for

Atmospheric Composition Change (NDACC) database is proposed. One essential aspect of the proposed approach is the propagation in parallel of all independent uncertainty components through the data processing chain before they are combined together to form the ozone combined standard uncertainty.
The independent uncertainty components contributing to the overall budget include random noise associated with signal detection, uncertainty due to saturation correction, background noise extraction, the absorption cross sections of O3, NO2 , SO2 , and O2 , the molecular extinction cross sections, and the number densities of the air, NO2, and SO2. The expression of the individual uncertainty components and their step-by-step propagation through the ozone differential absorption lidar (DIAL) processing chain are thoroughly estimated. All sources of uncertainty except detection noise imply correlated terms in the vertical dimension, which requires knowledge of the covariance matrix when the lidar signal is vertically filtered. In addition, the covariance terms must be taken into account if the same detection hardware is shared by the lidar receiver channels at the absorbed and non-absorbed wavelengths.
The ozone uncertainty budget is presented as much as possible in a generic form (i.e., as a function of instrument performance and wavelength) so that all ozone DIAL investigators can estimate, for their own instrument and in a straightforward manner, the expected impact of each reviewed uncertainty component.

6.2 Level of approximation

In what way is the uncertainty calculation procedure an approximation?

- *Is it based on (as is common practice) a first-order Taylor approximation (see GUM, Eq. (13))*

$$u_c^2(y) = \sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i, x_j) = \sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i, x_j)$$

  which will not be exact if f is nonlinear.
- *Are correlations between input quantities neglected?*
- *Other approximations?*

Answer:
The approach is rigorous. Assumptions have to be made in case e.g. certain system parameters are unknown.

If an approximation is involved, do you think the approximation can be a problem, or do you consider it justified?

Answer:
This depends on the application. For satellite (profile) validation the ozone DIAL systems have proven very adequate. Also, instrumental errors are known well enough to allow trend detection:

W. Steinbrecht, H. Claude, F. Scho¨nenborn, I. S. McDermid, T. Leblanc, S. Godin, T. Song, D. P. J. Swart, Y. J. Meijer, G. E. Bodeker, B. J. Connor, N. K˙ampfer, K. Hocke, Y. Calisesi, N. Schneider, J. de la No¨e, A. D. Parrish, I. S. Boyd, C. Bru¨hl, B. Steil, M. A. Giorgetta, E. Manzini, L. W.

Thomason, J. M. Zawodny, M. P. McCormick, J. M. Russell, P. K. Bhartia, R. S. Stolarski, and S. M. Hollandsworth-Frith. Long-term evolution of upper stratospheric ozone at selected stations of the network for the detection of stratospheric change (NDSC). *Journal of Geophysical Research: Atmospheres*, 111(D10):n/a–n/a, 2006. D10308.

7. Uncertainty contributions

7.1 Prior

Is there a prior contribution? If so, is this prior based on measured data, a model, a rough guess, or something else?

Answer: Absorption cross sections are externally measured.

7.2 Smoothing error

Is an error source "smoothing error" included in the uncertainty calculation? If so, what do you define as "smoothing error"? Should the averaging kernel of the data product be applied in some way, before the uncertainty can be properly interpreted?

Answer:
Smoothing errors and the effect on resolution and uncertainty are extensively described in:

Leblanc, T., Sica, R. J., van Gijsel, J. A. E., Godin-Beekmann, S., Haefele, A., Trickl, T., Payen, G., and Gabarrot, F.: Proposed standardized definitions for vertical resolution and uncertainty in the NDACC lidar ozone and temperature algorithms – Part 1: Vertical resolution, Atmos. Meas. Tech., 9, 4029-4049, doi:10.5194/amt-9-4029-2016, 2016.

7.3 Noise

Is there a noise contribution? If so, what do you define as "noise"? (E.g., for MOPITT, one considers an instrumental noise, but also a "geophysical noise" (Deeter, 2013).)

Answer:
Yes, this is due to the background noise measured on each single or integrated lidar signal before the processing, subtracted in according to the solution of the lidar equation (see term P_B in Eq.1). In addition, the noise due to dark currents (instrumental noise due to the electronics), which provides a sort bias on the collected signal in analog detection mode, is measured before or after each measurement session by obscuring the instrument receiver and is then subtracted from the signals during the signal processing.

7.4 Random and systematic contributions

Do you consider explicitly separately "random", "structured random" and "systematic" contributions? If so, how do you define each of these in your calculation?

Answer:
Random:
The independent uncertainty components contributing to the overall budget include random noise associated with signal detection, uncertainty due to saturation correction, background noise extraction

Structured random:
Number densities of the air, NO2, and SO2, aerosols

Systematic:
The absorption cross sections of O3, NO2 , SO2 , and O2 , the molecular extinction cross sections

7.5 Input quantities / other parameters

If the main measured quantities of the data product depend on input quantities, how do the final uncertainties depend on uncertainties of these input quantities? Please provide a list with input quantities of which the uncertainties:

1. *Are taken into account.*
2. *Could be important, but are not taken into account. For example, because their consideration would be technically difficult, or it is not clear how to estimate the associated uncertainty.*
3. *Are not taken into account, as they can be demonstrated to be negligible.*

If this list is already available somewhere in a literature source, you can simply refer to it.

Input quantity/other parameter	associated uncertainty or “important but ignored” or “negligible”	Extra info (e.g., random, systematic)
Absorption cross section	Important	systematic
Number densities	Important	Structured random
Aerosol homogeneity	Important	Structured random

7.6 Uncertainty due to model error

Do you consider explicitly an uncertainty contribution due to the fact that the model is not perfect? Such uncertainty can be revealed e.g., by comparing results of several retrieval models.

Answer:
See above the description at section 7.4 of the error associated with the estimate of temperature and pressure profiles. In particular for tropospheric ozone, the vertical distribution of aerosols has an important impact on the retrieved ozone profile.

8. Correlations/covariances

8.1 Presence in data product

Do you provide correlations or covariances within your data product, directly relevant to the main measured quantity? If so, between which quantities?

Answer:
No. As mentioned above each profile is accompanied by profiles indicating the effective vertical resolution which is the result of the applied smoothing filtering. The related covariance matrix is not provided but can be calculated from the smoothing data.

8.2 Auto-correlation

Suppose a user has to average several measured values of your data product. E.g., they want the mean column, 100 km around the observation site, within one month. Can you give a recommendation how they can obtain the uncertainty of this mean column, starting from the uncertainties provided for the individual columns?

Answer: N/A

8.3 Correlation between main measured quantity and other quantities

Do you provide any correlation info between the main measured quantity (e.g., an ozone profile) and other quantities (e.g., a temperature profile)?

Answer:
There are interdependencies of the retrieved ozone profile with the presence of aerosol. These effects are described the following paper:

E. V. Browell, S. Ismail, and S. T. Shipley. Ultraviolet DIAL Measurements of O3 Profiles in Regions of Spatially Inhomogeneous Aerosols. *Appl. Opt.*, 24:2827–2836, 1985.

9. Bias handling introduced during processing

Biases can, at least in theory, be introduced during processing. For example by nonlinear measurement equations in combination with large uncertainties on the input quantities. Is this something you try to correct for, or report, or deal with in some other way? Or do you think this will be negligible?

Answer:
This bias is due the error introduced by data-handling procedures such as signal averaging during varying atmospheric extinction and scattering conditions.

10. Other remarks on data product uncertainty

Please put here any other information about the data product uncertainty that you think is important.

Annex D

GAIA-CLIM questionnaire about uncertainty in data products

Lidar – Temperature profiles

Table of Contents

1. Identification of respondent and of data product

What are your contact details?

Answer:

Arnoud Apituley
KNMI - Royal Netherlands Meteorological Institute
P.O. Box 201, 3730 AE De Bilt
Ph: +31 6 55457540
apituley@knmi.nl

For which data product are you filling in this questionnaire?

Answer: Temperature lidar

Please provide one or more accessible sources of information that a non-expert user can refer to, to gain an understanding of the measurement technique.

Answer:

Wandinger, U., 2005: Introduction to lidar. Lidar: Range-Resolved Optical Remote Sensing of the Atmosphere, C. Weitkamp, Ed., Springer Series of Optical Sciences, Vol. 102, Springer, Chapter 1, pp 1–18.

2. Recommended literature

*Which literature work would you recommend to understand better the measurement technique and the **general uncertainty framework** within which uncertainties of the data product are constructed. Note that for metrology, the vocabulary list of the VIM (*International Vocabulary of Metrology*), and the uncertainty framework of the GUM (Guide to expression of uncertainty) are important standards. Please provide a complete reference or doi where possible.*

Answer:

Wandinger, U., 2005: Introduction to lidar. Lidar: Range-Resolved Optical Remote Sensing of the Atmosphere, C. Weitkamp, Ed., Springer Series of Optical Sciences, Vol. 102, Springer, Chapter 1, pp 1–18.

*More specifically, which literature works (article, ATBD, other…) would you recommend to understand better how uncertainties of **this particular data product** are conceived? Please provide a complete reference or doi where possible.*

Answer:

E. D. Hinkley. *Laser monitoring of the atmosphere*. Springer Verlag, Berlin, 1976.

Behrendt., 2005: Introduction to lidar. Lidar: Range-Resolved Optical Remote Sensing of the

Atmosphere, C. Weitkamp, Ed., Springer Series of Optical Sciences, Vol. 102, Springer, Chapter 10, 'Temperature Measurements with Lidar, pp 273–300.

A. Hauchecorne and M.L. Chanin. Density and temperature profiles obtained by lidar between 35 and 70 km. *Geophys. Res. Lett.*, 7(8):565–568, Aug 1980.

T. Leblanc, R. J. Sica, J. A. E. van Gijsel, A. Haefele, G. Payen, and G. Liberti. Proposed standardized definitions for vertical resolution and uncertainty in the NDACC lidar ozone and temperature algorithms – Part 3: Temperature uncertainty budget. *Atmospheric Measurement Techniques*, 9(8):4079–4101, 2016.

3. Main measured quantity (measurand)

3.1 Specification of measurand

Specify the main measured quantities (i.e., the measurands) and the associated unit of the data product, along with their field name in the data product

Example measurands with unit: Temperature [K], O3 profile [ppmv], water vapour [ppmv]

3.2 Measurement equation

What is the relation between the main measured quantity of the data product and input quantities? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to literature publications).

Answer:
As in most lidar applications, the fundamental equation at the source of the middle atmospheric temperature lidar retrieval using the density integration technique is the lidar equation (e.g., Hinkley, 1976). The equation describes the emission of light by a laser source, its backscatter at altitude z, its extinction and scattering along the laser beam path up and back, and its collection on a detector. One form of the lidar equation is expressed as:

$$P(z,\lambda_1,\lambda_2) = P_L(\lambda_1)\frac{\eta(z,\lambda_2)\delta z}{(z-z_L)^2}\tau_{UP}(z,\lambda_1)\beta(z,\lambda_1,\lambda_2)\tau_{DOWN}(z,\lambda_2), \quad (3)$$

- z is the altitude of the backscattering layer;
- z_L is the altitude of the lidar (laser and receiver assumed to be at the same altitude);
- β is the total backscatter coefficient (including particulate and molecular backscatter);
- τ_{UP} is the atmospheric transmission integrated along the outgoing beam path between the lidar and the scattering altitude z, and is defined as

$$\tau_{UP}(z) = \exp \left[-\int_{z_L}^{z} \left(\sigma_M(\lambda_1) N_a(z') + \alpha_P(z', \lambda_1) + \sum_i \sigma_i(z', \lambda_1) N_i(z') \right) dz' \right]; \quad (4)$$

- τ_{DOWN} is the atmospheric transmission integrated along the returning beam path between the scattering altitude z and the lidar receiver, and is defined as

$$\tau_{DOWN}(z) = \exp \left[-\int_{z_L}^{z} \left(\sigma_M(\lambda_2) N_a(z') + \alpha_P(z', \lambda_2) + \sum_i \sigma_i(z', \lambda_2) N_i(z') \right) dz' \right], \quad (5)$$

where σ_M is the molecular extinction cross section due to Rayleigh scattering (Strutt, 1899) (hereafter called "Rayleigh cross section" for brevity), N_a is the air number density, α_P is the particulate extinction coefficient, σ_i is the absorption cross section of absorbing constituent i, and N_i is the number density of absorbing constituent i. For altitudes between the ground and 90 km, the Rayleigh cross sections can be considered constant with altitude, and therefore depend only on wavelength. The absorption cross sections, however, are in most cases temperature-dependent, and should be taken as a function of both altitude and wavelength. Temperature is retrieved by inverting Eq. (3) with respect to the backscatter term β.

In the absence of particulate backscatter, the backscatter coefficient β, and therefore the lidar signal collected on the detector, is proportional to the air number density. Temperature is then calculated by vertically integrating air number density, assuming hydrostatic balance and assuming that the air is an ideal gas (Hauchecorne and Chanin, 1980). This inversion technique works for both elastic scattering (Rayleigh backscatter by the air molecules) and inelastic scattering (normally, using vibrational Raman backscatter by the nitrogen molecules) (Strauch et al., 1971; Gross et al., 1997). For either technique, we can write a generic form of the backscatter coefficient as a function of air number density N_a:

$$\beta(z) = \sigma_\beta N_a(z). \tag{6}$$

For Rayleigh backscatter, the effective cross section σ_β is the molecular (Rayleigh) scattering cross section at the emission wavelength λ_1:

$$\sigma_\beta = \sigma_M(\lambda_1). \tag{7}$$

For Raman backscatter, the effective cross section σ_β is the vibrational Raman scattering cross section of a well-mixed gas (typically nitrogen) at the Raman-shifted wavelength λ_2, multiplied by the mixing ratio of the well-mixed gas (e.g., 0.781 for nitrogen):

$$\sigma_\beta = 0.781\sigma_{N2}(\lambda_1, \lambda_2). \tag{8}$$

Substituting into the lidar equation Eq. (3), we obtain an expression of air number density as a function of the backscatter lidar signal:

$$N_a(z) = \frac{P(z, \lambda_1, \lambda_2)(z - z_L)^2}{\sigma_\beta \eta(z, \lambda_1, \lambda_2)\delta z P_L(\lambda_1)\tau_{UP}(z, \lambda_1)\tau_{DOWN}(z, \lambda_2)}. \tag{9}$$

A temperature profile is then calculated, assuming hydrostatic balance, and assuming that the air is an ideal gas with a constant mean molecular mass:

$$T(z - \delta z) = \frac{N_a(z)}{N_a(z - \delta z)} T(z) + \frac{M_a}{R_a N_a(z - \delta z)} \overline{N_a}(z)\overline{g}(z)\delta z, \tag{10}$$

where T is the retrieved temperature, M_a is the molecular mass of dry air, R_a is the ideal gas constant, and g is the acceleration of gravity. The horizontal bar above N_a and g represents the average value of N_a and g between z and $z - \delta z$. An essential aspect of the method is that all altitude-independent terms (e.g., Rayleigh cross section, lidar receiver efficiency) cancel out when computing the ratio of air number density at altitudes z and $z - \delta z$.

Starting from the top of the profile z(kTOP) where temperature is initialized using an ancillary temperature measurement Ta (kTOP) (procedure called temperature “tie-on”), the complete temperature profile can be retrieved integrating downward using lidar-measured relative number density.

4. Traceability and comparability

4.1 SI or community traceability

Is the measurement quantity traceable, via an unbroken chain of processing steps, to SI units or community accepted standards?

Answer: Yes.

If yes, please provide references to available literature describing the traceability aspects of the measurement.

T. Leblanc, R. J. Sica, J. A. E. van Gijsel, A. Haefele, G. Payen, and G. Liberti. Proposed standardized definitions for vertical resolution and uncertainty in the NDACC lidar ozone and temperature algorithms – Part 3: Temperature uncertainty budget. *Atmospheric Measurement Techniques*, 9(8):4079–4101, 2016.

If no, please describe what aspects of the measurement are not fully traceable and how this aspect is addressed in deriving the data product and its uncertainty.

4.2 Comparability

If measurements are taken at multiple sites, are efforts made to ensure sufficiently similar measurement technique approaches to ensure comparability? Please provide links to any supporting materials available such as instrument manuals / network protocols.

Answer: Yes.

In NDACC, regular intercomparisons are carried out between temperature lidar systems for stratospheric temperature. These systems are often also systems for stratospheric ozone, e.g.:

Philippe Keckhut, Stuart McDermid, Daan Swart, Thomas McGee, So- phie Godin-Beekmann, Alberto Adriani, John Barnes, Jean-Luc Baray, Hassan Bencherif, Hans Claude, Aleide G. di Sarra, Georgio Fiocco, Georg Hansen, Alain Hauchecorne, Thierry Leblanc, Choo Hie Lee, Shiv Pal, Gerard Megie, Hideaki Nakane, Roland Neuber, Wolfgang Steinbrecht, and Jeffrey Thayer. Review of ozone and temperature lidar validations performed within the framework of the network for the detection of stratospheric change. J. Environ. Monit., 6:721–733, 2004.

Upendra N. Singh, Philippe Keckhut, Thomas J. McGee, Michael R. Gross, Alain Hauchecorne, Evan F. Fishbein, Joe W. Waters, John C. Gille, Aidan E. Roche, and James M. Russell. Stratospheric temperature measurements by two collocated NDSC lidars during UARS validation campaign. *Journal of Geophysical Research: Atmospheres*, 101(D6):10287– 10297, 1996.

Steinbrecht, W., McGee, T. J., Twigg, L. W., Claude, H., Schönenborn, F., Sumnicht, G. K., and Silbert, D.: Intercomparison of stratospheric ozone and temperature profiles during the October 2005 Hohenpeißenberg Ozone Profiling Experiment (HOPE), Atmos. Meas. Tech., 2, 125-145, doi:10.5194/amt-2-125-2009, 2009.

5. Representation of the uncertainty in the data product

5.1 Uncertainty field name(s)

Which field name(s) are used in the data product to hold the uncertainty value(s) associated with the main measured quantities? Note that more than one uncertainty field name can be associated with a single quantity (e.g., one field name for the "uncertainty due to random effects" and one for the "uncertainty due to systematic effects").

Field name of uncertainty	Associated quantity
Error	Random uncertainty

5.2 Uncertainty form

In what form is the uncertainty per measurement represented in the data product? For example, is it:

- *A standard uncertainty (i.e., uncertainty expressed as standard deviation)*
- *A 95% coverage interval*
- *A variance-covariance matrix (if so, explain between which quantities the covariance is taken into account)*
- *A probability density function*
- *Other [please specify]*

Answer:
Standard uncertainty (i.e., uncertainty expressed as standard deviation) with respect to the random error in the lidar signals.

6. Uncertainty calculation

6.1 Formula/procedure

What is the formula/procedure by which the uncertainty is calculated? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to one or more equations in the literature).

Answer:

The background and procedures are described in:

T. Leblanc, R. J. Sica, J. A. E. van Gijsel, A. Haefele, G. Payen, and G. Liberti. Proposed standardized definitions for vertical resolution and uncertainty in the NDACC lidar ozone and temperature algorithms – Part 3: Temperature uncertainty budget. *Atmospheric Measurement Techniques*, 9(8):4079–4101, 2016.

Is the uncertainty obtained by:

- *Uncertainty propagation, taking into account the uncertainties of the input quantities,*
- *Probability density function propagation,*
- *Sensitivity analysis: i.e., varying parameters and check the impact on the output quantity,*
- *Or still some other procedure?*

Answer:
One important aspect of the proposed approach is the ability to propagate all independent uncertainty components in parallel through the data processing chain. The individual uncertainty components are then combined at the very last stage of processing to form the temperature combined standard uncertainty.
The identified uncertainty sources comprise major components such as signal detection, saturation correction, back- ground noise extraction, temperature tie-on at the top of the profile, and absorption by ozone if working in the visible spectrum, as well as other components such as molecular extinction, the acceleration of gravity, and the molecular mass of air, whose magnitudes depend on the instrument, data pro- cessing algorithm, and altitude range of interest. The expression of the individual uncertainty components and their step-by-step propagation through the temperature data processing chain are thoroughly estimated, taking into account the effect of vertical filtering and the merging of multiple channels. All sources of uncertainty except detection noise imply correlated terms in the vertical dimension, which means that covariance terms must be taken into account when vertical filtering is applied and when temperature is integrated from the top of the profile. Quantitatively, the uncertainty budget is presented in a generic form (i.e., as a function of instrument performance and wavelength), so that any NDACC temperature lidar investigator can easily estimate the expected impact of individual uncertainty components in the case of their own instrument.

6.2 Level of approximation

In what way is the uncertainty calculation procedure an approximation?

- *Is it based on (as is common practice) a first-order Taylor approximation (see GUM, Eq. (13))*

$$u_c^2(y) = \sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i, x_j) = \sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i, x_j)$$

  which will not be exact if f is nonlinear.
- *Are correlations between input quantities neglected?*
- *Other approximations?*

Answer:
The approach is rigorous. Assumptions have to be made in case e.g. certain system parameters are unknown.

If an approximation is involved, do you think the approximation can be a problem, or do you consider it justified?

Answer: Approximations are justified.

7. Uncertainty contributions

7.1 Prior

Is there a prior contribution? If so, is this prior based on measured data, a model, a rough guess, or something else?

Answer:
Starting from the top of the profile z(kTOP) where temperature is initialized using an ancillary temperature measurement Ta (kTOP) (procedure called temperature “tie-on”), the complete temperature profile can be retrieved integrating downward using lidar-measured relative number density.

7.2 Smoothing error

Is an error source “smoothing error” included in the uncertainty calculation? If so, what do you define as “smoothing error”? Should the averaging kernel of the data product be applied in some way, before the uncertainty can be properly interpreted?

Answer:
Smoothing errors and the effect on resolution and uncertainty are extensively described in:

Leblanc, T., Sica, R. J., van Gijsel, J. A. E., Godin-Beekmann, S., Haefele, A., Trickl, T., Payen, G., and Gabarrot, F.: Proposed standardized definitions for vertical resolution and uncertainty in the NDACC lidar ozone and temperature algorithms – Part 1: Vertical resolution, Atmos. Meas. Tech., 9, 4029-4049, doi:10.5194/amt-9-4029-2016, 2016.

7.3 Noise

Is there a noise contribution? If so, what do you define as “noise”? (E.g., for MOPITT, one considers an instrumental noise, but also a “geophysical noise” (Deeter, 2013).)

Answer:
Yes, this is due to the background noise measured on each single or integrated lidar signal before the processing, subtracted in according to the solution of the lidar equation. In addition, the noise due to dark currents (instrumental noise due to the electronics), which provides a sort bias on the collected signal in analog detection mode, is measured before or after each measurement session by obscuring the instrument receiver and is then subtracted from the signals during the signal processing.

7.4 Random and systematic contributions

Do you consider explicitly separately “random”, “structured random” and “systematic” contributions? If so, how do you define each of these in your calculation?

Answer:
Random: The independent uncertainty components contributing to the overall budget include random noise associated with signal detection, uncertainty due to saturation correction, background noise extraction.

7.5 Input quantities / other parameters

If the main measured quantities of the data product depend on input quantities, how do the final uncertainties depend on uncertainties of these input quantities? Please provide a list with input quantities of which the uncertainties:

1. *Are taken into account.*
2. *Could be important, but are not taken into account. For example, because their consideration would be technically difficult, or it is not clear how to estimate the associated uncertainty.*
3. *Are not taken into account, as they can be demonstrated to be negligible.*

If this list is already available somewhere in a literature source, you can simply refer to it.

Input quantity/other parameter	associated uncertainty or “important but ignored” or “negligible”	Extra info (e.g., random, systematic)
Tie-on Temperature		
Aerosol homogeneity	Important	Structured random

7.6 Uncertainty due to model error

Do you consider explicitly an uncertainty contribution due to the fact that the model is not perfect? Such uncertainty can be revealed e.g., by comparing results of several retrieval models.

Answer:
Several assumptions about the properties of the atmosphere must be made to help reduce the complexity of our proposed measurement model. This is extensively described in:

T. Leblanc, R. J. Sica, J. A. E. van Gijsel, A. Haefele, G. Payen, and G. Liberti. Proposed standardized definitions for vertical resolution and uncertainty in the NDACC lidar ozone and temperature algorithms – Part 3: Temperature uncertainty budget. *Atmospheric Measurement Techniques*, 9(8):4079–4101, 2016.

8. Correlations/covariances

8.1 Presence in data product

Do you provide correlations or covariances within your data product, directly relevant to the main measured quantity? If so, between which quantities?

Answer: Yes. Temperature and pressure.

8.2 Auto-correlation

Suppose a user has to average several measured values of your data product. E.g., they want the mean column, 100 km around the observation site, within one month. Can you give a recommendation how they can obtain the uncertainty of this mean column, starting from the uncertainties provided for the individual columns?

Answer: N/A

8.3 Correlation between main measured quantity and other quantities

Do you provide any correlation info between the main measured quantity (e.g., an ozone profile) and other quantities (e.g., a temperature profile)?

Answer:
There are interdependencies of the retrieved temperature profile with the presence of aerosol.

9. Bias handling introduced during processing

Biases can, at least in theory, be introduced during processing. For example by nonlinear measurement equations in combination with large uncertainties on the input quantities. Is this something you try to correct for, or report, or deal with in some other way? Or do you think this will be negligible?

Answer:
Errors which are caused by the initialization were investigated for downward integration using simulated data which were 15 K above the model atmosphere for all heights. It was found that the 15 K initialization error at 90km decreased to 4 K at 80km and to 1 K at 70 km. For real measurements the reference-height value should be much closer to the correct data than in this worst-case scenario so the actual downward-integration errors should be considerably smaller. It must be noted in this context that, when a systematic error in the form of altitude-dependent signal-induced noise is present in the signals, inaccurate background subtraction can cause large errors. Signal-induced noise, when present, must be identified, and the data must be corrected.

10. Other remarks on data product uncertainty

Please put here any other information about the data product uncertainty that you think is important.

Annex E

GAIA-CLIM questionnaire about uncertainty in data products

MWR – Water vapour profiles

Table of contents

1. Identification of respondent and of data product

What are your contact details?

Answer:

Domenico Cimini
National Research Council of Italy – Institute of Methodologies for Environmental Monitoring (CNR-IMAA)
C.da S.Loja, 85050, Tito Scalo, Potenza
Phone: +39/3311706062
E-mail: domenico.cimini@imaa.cnr.it

For which data product are you filling in this questionnaire?

Answer:
Atmospheric humidity profiles from ground-based microwave radiometer (MWR)

Please provide one or more accessible sources of information that a non-expert user can refer to, to gain an understanding of the measurement technique.

Answer:
EU COST EG-CLIMET Final report – MWR Section:
http://cfa.aquila.infn.it/wiki.eg-climet.org/index.php5/Microwave_radiometer
MWR on Wikipedia (prepared by ITARS fellows, itars.uni-koeln.de):
https://en.wikipedia.org/wiki/Microwave_radiometer

2. Recommended literature

*Which literature work would you recommend to understand better the measurement technique and the **general uncertainty framework** within which uncertainties of the data product are constructed. Note that for metrology, the vocabulary list of the VIM (*International Vocabulary of Metrology*), and the uncertainty framework of the* GUM (Guide to expression of uncertainty) are important standards. Please provide a complete reference or doi where possible.

Answer:

Han, Y. and E. R. Westwater (2000), Analysis and Improvement of Tipping Calibration for Ground-based Microwave Radiometers. IEEE Trans. Geosci. Remote Sens., 38(3), 1260–127, doi: 10.1109/36.843018.

Hewison, T. (2006), Profiling Temperature and Humidity by Ground-based Microwave Radiometers, PhD Thesis, University of Reading. Online: http://tim.hewison.org/Thesis.pdf

Küchler, N., D. D. Turner, U. Löhnert, and S. Crewell (2016), Calibrating ground-based microwave radiometers: Uncertainty and drifts, Radio Sci., 51, 311–327, doi:10.1002/2015RS005826.

Maschwitz, G., U. Löhnert, S. Crewell, T. Rose, and D. Turner (2013), Investigation of ground-based microwave radiometer calibration techniques at 530 hPa, Atm. Meas. Tech., 6, 2641–2658, doi:10.5194/amt-6-2641-2013.

Rodgers, C.D. (2000), Inverse Methods for Atmospheric Sounding: Theory and Practice, World Scientific Publishing Co. Ltd. ISBN: 978-981-02-2740-1

More specifically, which literature works (article, ATBD, other…) would you recommend to understand better how uncertainties of this particular data product are conceived? Please provide a complete reference or doi where possible.

Answer:

Cadeddu, M. P., Liljegren, J. C., and Turner, D. D. (2013), The Atmospheric radiation measurement (ARM) program network of microwave radiometers: instrumentation, data, and retrievals, Atmos. Meas. Tech., 6, 2359-2372, doi:10.5194/amt-6-2359-2013.

Cimini, D., T. J. Hewison, L. Martin, J. Güldner, C. Gaffard and F. S. Marzano (2006), Temperature and humidity profile retrievals from ground-based microwave radiometers during TUC, Met. Zeitschrift, 15, 1, 45-56, doi: 10.1127/0941-2948/2006/0099.

Cimini D., E. Campos, R. Ware, S. Albers, G. Giuliani, J. Oreamuno, P. Joe, S. Koch, S. Cober, and E. Westwater (2011), Thermodynamic Atmospheric Profiling during the 2010 Winter Olympics Using Ground-based Microwave Radiometry, IEEE Trans. Geosci. Rem. Sens., 49, 12, 4959-4969. doi: 10.1109/TGRS.2011.2154337.

Löhnert, U. and O. Maier (2012), Operational profiling of temperature using ground-based microwave radiometry at Payerne: prospects and challenges, Atmos. Meas. Tech., 5, 1121-1134, doi:10.5194/amt-5-1121-2012.

Maschwitz, G. (2012), Assessment of Ground-Based Microwave Radiometer Calibration to Enable Investigation of Gas Absorption Models. PhD thesis, Universität zu Köln. Online: http://kups.ub.uni-koeln.de/5390/1/DissertationGerritMaschwitz.pdf

Hewison, T. (2007), 1D-VAR retrievals of temperature and humidity profiles from a ground-based microwave radiometer, IEEE Trans. Geosci. Rem. Sens., 45, 7, 2163-2168, doi: 10.1109/TGRS.2007.898091.

Please specify also if the literature source is still up-to-date with the current data product. If not, where can a user find the information on the latest version of the data product and its uncertainties?

Answer:

Most of the current MWR data products do not include uncertainties. Exceptions are the MWR products produced by the ARM Program (Atmospheric Measurement Program, www.arm.gov) and by the HD(CP)^2 project (High Definition Clouds and Precipitation for Climate Prediction, https://hdcp2.zmaw.de). Uncertainties in MWR derived products are usually estimated *ex ante* though simulated analysis (Cadeddu et al., 2013) or *ex post* through validation against collocated radiosonde profiles (Löhnert and Maier, 2012). Dynamical uncertainty estimates have been proposed (Hewison, 2007; Cimini et al., 2011) but have been so far computed for limited datasets (i.e. not operationally and for limited time periods and MWR units).

3. Main measured quantity (measurand)

3.1 Specification of measurand

Specify the main measured quantities (i.e., the measurands) and the associated unit of the data product, along with their field name in the data product

Example measurands with unit: Temperature [K], O3 profile [ppmv], water vapour [ppmv]

Quantity [unit]	Field name
Brightness Temperature [K]	tb
Atmospheric absolute humidity [kg m-3]	hua

3.2 Measurement equation

What is the relation between the main measured quantity of the data product and input quantities? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to literature publications).

Answer:
The primary measured quantity is downwelling brightness temperature (tb). Atmospheric absolute humidity (hua) is derived from tb through an inversion method, usually multivariate regression, neural network, or optimal estimation. These methods are described in Cimini et al. (2006). A brief summary is given below.

The primary observable tb is related to the atmospheric state through the radiative transfer equation, which can be written in its discrete form as:

$$\mathbf{y} = \mathbf{F}(\mathbf{x}) + \boldsymbol{\varepsilon}$$

where **y** is the measurement vector (tb and ancillary data), **x** is the atmospheric state vector (ta in this case), **F** is the operator relating the measurements to the unknown atmospheric state vector, and **ε** is the measurements uncertainty. A general solution is given by optimal estimation (Rodgers, 2000). For the linear case, the solution can be written as:

$$\hat{\mathbf{x}} = \mathbf{x}_{\mathrm{b}} + [\mathbf{B}^{-1} + \mathbf{K}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{K}]^{-1}\mathbf{K}^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{y} - \mathbf{K}\mathbf{x}_{\mathrm{b}})$$

If a priori data set of simultaneous **x** and **y** is available, this may be solved through multivariate linear regression:

$$\hat{\mathbf{x}} = \mathbf{x}_0 + \mathbf{C}_{\mathbf{xy}} \cdot \mathbf{C}_{\mathbf{yy}}{}^{-1}(\mathbf{y} - \mathbf{y}_0)$$

For moderately non-linear problems, the solution is achieved by iteration:

$$\hat{\mathbf{x}}_{i+1} = \hat{\mathbf{x}}_i + \left[\mathbf{B}^{-1} + \mathbf{K}_i^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{K}_i\right]^{-1} \cdot \left[\mathbf{K}_i^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{y} - F(\hat{\mathbf{x}}_i)) - \mathbf{B}^{-1}(\hat{\mathbf{x}}_i - \mathbf{x}_b)\right]$$

where:
y the measurement vector
$\mathbf{y}_0$ the mean measurement vector
x the atmospheric state vector
$\mathbf{x}_b$ the background (a priori) atmospheric state vector
$\mathbf{x}_0$ the mean atmospheric state vector
$\hat{\mathbf{x}}$ the estimated atmospheric state vector
K the Jacobian matrix of the observation vector with respect to the state vector
ε the measurements uncertainty
B the background (a priori) uncertainty covariance matrices

R the measurement uncertainty covariance matrices
$\mathbf{C_{xy}}$ the covariance matrix extracted from a priori data set of simultaneous **x** and **y**
$\mathbf{C_{yy}}$ the autocovariance matrix extracted from a priori data set of **y**

4. Traceability and comparability

4.1 SI or community traceability

Is the measurement quantity traceable, via an unbroken chain of processing steps, to SI units or community accepted standards?

Answer:
No at the present time. Traceability chains are available on www.gaia-clim.eu .

If yes, please provide references to available literature describing the traceability aspects of the measurement.

If no, please describe what aspects of the measurement are not fully traceable and how this aspect is addressed in deriving the data product and its uncertainty.

The following aspects are not fully traceable.

Target emissivity and temperature sensors
The MWR measurement traceability needs to be enforced in the calibration procedure (transfer from raw voltages to tb). This implies the use of certified black-body targets and temperature sensors (measuring the target temperature). Commercial black-body targets have reached a mature state, but the manufacturer's data are usually limited (e.g. 18 GHz is a typical maximum frequency even if the target is used above that frequency). Despite many realizations of microwave brightness temperature standards exist in the form of heated or cooled calibration targets, none are currently maintained as a national standard by a National Measurement Institute (NMI). Metrology applicable to microwave remote sensing radiometry is currently under development, including tb standards. It is expected that SI-traceable tb calibration for black-body targets and transfer standards in the form of calibrated black-body targets will be available in the next few years.
Currently the target emissivity is assumed to be unity within -40 dB (i.e. between 0.9999 and 1.0). The calibration error associated to that uncertainty should be negligible.

Absorption model
Absorption of radiation by atmospheric gases and hydrometeors is quantitatively modelled while solving the forward problem through the radiative transfer equation. Thus, absorption model uncertainties affect all the retrieval methods based on simulated brightness temperatures. Only retrieval methods based on historical datasets of MWR observations and simultaneous atmospheric soundings are not affected by absorption model uncertainties (e.g. measurement-based regression in Cimini et al., 2006).
A proper characterization of the absorption model contribution to the total uncertainty is lacking.

Currently, the absorption model uncertainty is estimated as the difference among existing most common absorption models.

4.2 Comparability

If measurements are taken at multiple sites, are efforts made to ensure sufficiently similar measurement technique approaches to ensure comparability? Please provide links to any supporting materials available such as instrument manuals / network protocols.

Answer:
Protocols to ensure sufficiently similar measurements have been developed by ARM (Cadeddu et al., 2013) and are currently applied for MWR measurements taken at their sites.
Similar efforts are carried out within TOPROF (www.toprof.eu) and previous EU COST actions, e.g. reports from the Joint Calibration Experiments (JCAL 1[1] and 2[2]) and MWRnet[3].

[1] http://tinyurl.com/JCAL1-report-pdf
[2] http://tinyurl.com/JCAL2-report-pdf
[3] http://cetemps.aquila.infn.it/mwrnet/main_files/reports.html

5. Representation of the uncertainty in the data product

5.1 Uncertainty field name(s)

Which field name(s) are used in the data product to hold the uncertainty value(s) associated with the main measured quantities? Note that more than one uncertainty field name can be associated with a single quantity (e.g., one field name for the "uncertainty due to random effects" and one for the "uncertainty due to systematic effects").

Field name of uncertainty	Associated quantity
offset_tb	brightness temperature offset subtracted from measured brightness temperature
tb_bias	systematic calibration uncertainty of brightness temperature, one standard deviation
tb_cov	error covariance matrix of brightness temperature channels
hua_offset	atmospheric absolute humidity offset correction based on brightness temperature offset
hua_err	standard error of atmospheric absolute humidity

5.2 Uncertainty form

In what form is the uncertainty per measurement represented in the data product? For example, is it:

- *A standard uncertainty (i.e., uncertainty expressed as standard deviation)*

- *A 95% coverage interval*
- *A variance-covariance matrix (if so, explain between which quantities the covariance is taken into account)*
- *A probability density function*
- *Other [please specify]*

Answer:
A standard uncertainty (i.e., uncertainty expressed as standard deviation)

6. Uncertainty calculation

6.1 Formula/procedure

What is the formula/procedure by which the uncertainty is calculated? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to one or more equations in the literature).

Answer:
When using regression, the estimated retrieval uncertainty is given as the standard deviation of the residuals ($\delta\mathbf{x} = \hat{\mathbf{x}} - \mathbf{x}_{true}$), i.e. the difference between the estimated ($\hat{\mathbf{x}}$) and the true ($\mathbf{x}_{true}$) atmospheric states for each member of the a priori data set:

$$u(\mathbf{x}) = \mathbf{std}(\delta\mathbf{x}) = \mathbf{std}(\hat{\mathbf{x}} - \mathbf{x}_{true})$$

When using an optimal estimation method, the estimated retrieval uncertainty is given by the diagonal terms of the posterior covariance matrix (same notation as 3.2 above):

$$\mathbf{S}_i = \left[\mathbf{B}^{-1} + \mathbf{K}_i^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{K}_i\right]^{-1}$$

$$u(\mathbf{x}) = \mathbf{diag}(\mathbf{S}_i)$$

Is the uncertainty obtained by:

- *Uncertainty propagation, taking into account the uncertainties of the input quantities,*
- *Probability density function propagation,*
- *Sensitivity analysis: i.e., varying parameters and check the impact on the output quantity,*
- *Or still some other procedure?*

Answer:
For tb, the uncertainty is estimated through sensitivity analysis (Maschwitz, 2012).
For the atmospheric retrieval (in this case the atmospheric absolute humidity hua), the uncertainty is estimated through

- when using regression: the standard deviation of the residuals from the a priori data set;
- when using optimal estimation method: uncertainty propagation (optimal estimation formalism; Rodgers, 2000).

6.2 Level of approximation

In what way is the uncertainty calculation procedure an approximation?

- *Is it based on (as is common practice) a first-order Taylor approximation (see GUM, Eq. (13))*

$$u_c^2(y) = \sum_{i=1}^{N}\sum_{j=1}^{N} \frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j} u(x_i, x_j) = \sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j} u(x_i, x_j)$$

which will not be exact if f is nonlinear.

- *Are correlations between input quantities neglected?*
- *Other approximations?*

Answer:
The uncertainty calculation is based on a first-order Taylor approximation.
Correlation between simultaneous measurements at different channels is usually neglected.

If an approximation is involved, do you think the approximation can be a problem, or do you consider it justified?

Answer:
The problem is moderately non-linear (Rodgers, 2000).
Investigation on the covariance matrix of simultaneous measurements at different channels shows small off-diagonal terms.
Thus, the above approximations are considered justified.

7. Uncertainty contributions

7.1 Prior

Is there a prior contribution? If so, is this prior based on measured data, a model, a rough guess, or something else?

Answer:
Atmospheric MWR radiometry is an ill-posed problem and thus prior information is essentials for constraining the solution. Usually prior information comes from either a climatological mean of measured data (e.g. radiosondes) or the output of an atmospheric model (e.g. analysis).
In the first case, the climatological mean, the uncertainty of the prior is estimated as the standard deviation of the measured dataset (e.g. multi-year radiosonde ensemble).
In the other case, the atmospheric model output, the uncertainty of the prior is estimated as the model background error covariance matrix.

7.2 Smoothing error

Is an error source "smoothing error" included in the uncertainty calculation? If so, what do you define as "smoothing error"? Should the averaging kernel of the data product be applied in some way, before the uncertainty can be properly interpreted?

Answer:
The smoothing error is part of the total uncertainty estimated with the optimal estimation method.

The smoothing error is defined as $(\mathbf{A}-\mathbf{I})(\mathbf{x}-\mathbf{x_b})$ whose covariance is $\mathbf{S}_\mathrm{S} = (\mathbf{A}-\mathbf{I})\mathbf{B}(\mathbf{A}-\mathbf{I})^T$ (Rodgers 2000, Section 3), where **A** is the averaging kernel matrix:

$$\mathbf{A}_i = \left[\mathbf{B}^{-1} + \mathbf{K}_i^\mathrm{T}\mathbf{R}^{-1}\mathbf{K}_i\right]^{-1}\mathbf{K}_i^\mathrm{T}\mathbf{R}^{-1}\mathbf{K}_i$$

Thus, if the smoothing error needs to be separated from the total uncertainty, the averaging kernel matrix **A** is needed. This is currently not provided in the data files. However, the averaging kernel matrix may be provided in the future, either computed from the optimal estimation formalism above or through a brute force approach (Löhnert and Maier, 2012).

7.3 Noise

Is there a noise contribution? If so, what do you define as "noise"? (E.g., for MOPITT, one considers an instrumental noise, but also a "geophysical noise" (Deeter, 2013).)

Answer:
Instrumental noise is considered as the random uncertainty affecting tb observations (i.e. radiometric noise).
Geophysical noise in this context may be interpreted to be the "representativeness error", i.e. the uncertainty deriving from the background spatial/temporal variability at the place/time of its use. This contribution represents the uncertainty in the generalized interpolation from background to observations (Hewison, 2007) and thus it is time variant and depends on atmospheric conditions. This contribution is currently not considered. It may be considered in the future as a contribution to the background or measurement covariance matrices, depending on its used definition.

7.4 Random and systematic contributions

Do you consider explicitly separately "random", "structured random" and "systematic" contributions? If so, how do you define each of these in your calculation?

Answer:
Random uncertainty for tb and hua are considered. Systematic calibration uncertainty for tb is considered. Systematic uncertainty of atmospheric absorption model is currently neglected (it may be considered in the future).

7.5 Input quantities / other parameters

If the main measured quantities of the data product depend on input quantities, how do the final uncertainties depend on uncertainties of these input quantities? Please provide a list with input quantities of which the uncertainties:

1. *Are taken into account.*
2. *Could be important, but are not taken into account. For example, because their consideration would be technically difficult, or it is not clear how to estimate the associated uncertainty.*
3. *Are not taken into account, as they can be demonstrated to be negligible.*

If this list is already available somewhere in a literature source, you can simply refer to it.

Input quantity/other parameter	associated uncertainty or “important but ignored” or “negligible”	Extra info (e.g., random, systematic)
prior	**B** (see equations above)	random
tb	tb_cov, tb_bias	random, systematic
forward model	Potentially important but ignored	systematic (most probably)
target emissivity	Negligible (if the claimed specification for target reflectivity (-40dB) are verified)	systematic

7.6 Uncertainty due to model error

Do you consider explicitly an uncertainty contribution due to the fact that the model is not perfect? Such uncertainty can be revealed e.g., by comparing results of several retrieval models.

Answer:
Absorption model uncertainty shall be considered. This is currently estimated by differences among most used existing absorption models. A proper estimate should consider the sensitivity to forward model parameter uncertainty.

8. Correlations/covariances

8.1 Presence in data product

Do you provide correlations or covariances within your data product, directly relevant to the main measured quantity? If so, between which quantities?

Answer:
The covariance between measurements at different channels is provided in the data files (tb_cov). When using optimal estimation method, the diagonal terms of the posterior covariance matrix are provided in the data files (hua_err). If required, the full posterior covariance matrix could be provided.

Please state in the table below which of the quantities are reported and/or included in the total error. Please use either yes, no or N/A for the first 2 columns and a short explanation in the 3rd. column. Add other quantities as relevant.

Quantity	Explicitly reported	Included in total error	Where reported / name given / comments
measurement noise covariance matrix	Yes	Yes	This is **R** in 3.2 and tb_cov in 5.1
a priori covariance matrix	No	Yes	This is **B** in 3.2

a posteriori covariance matrix	No	Yes	This is **S** in 6.1

8.2 Auto-correlation

Suppose a user has to average several measured values of your data product. E.g., they want the mean column, 100 km around the observation site, within one month. Can you give a recommendation how they can obtain the uncertainty of this mean column, starting from the uncertainties provided for the individual columns?

Answer:
The uncertainty of the average product may be estimated from the standard deviation of the averaged sample. This unlikely happens to be smaller than the average of the individual uncertainties, but in such a case I would suggest to take the latter as the uncertainty estimate.

8.3 Correlation between main measured quantity and other quantities

Do you provide any correlation info between the main measured quantity (e.g., an ozone profile) and other quantities (e.g., a temperature profile)?

Answer: No.

9. Bias handling introduced during processing

Biases can, at least in theory, be introduced during processing. For example by nonlinear measurement equations in combination with large uncertainties on the input quantities. Is this something you try to correct for, or report, or deal with in some other way? Or do you think this will be negligible?

Answer:
Biases are introduced by calibration and forward model uncertainties. Bias correction on tb is provided for some sites (offset_tb). The propagation of this bias onto retrieved atmospheric absolute humidity may also be provided (hua_offset).

10. Other remarks on data product uncertainty

Please put here any other information about the data product uncertainty that you think is important.

Since MWRnet is an unfunded, bottom-up network, different levels of characterization are currently available among members. A common processing would significantly reduce this heterogeneity; activities towards this goal are ongoing but may not be totally implemented within the available dataset.

Annex F

GAIA-CLIM questionnaire about uncertainty in data products

MWR – Temperature profiles

Table of Contents

1. Identification of respondent and of data product

What are your contact details?

Answer:

Domenico Cimini
National Research Council of Italy – Institute of Methodologies for Environmental Monitoring (CNR-IMAA)
C.da S.Loja, 85050, Tito Scalo, Potenza
Phone: +39/3311706062
E-mail: domenico.cimini@imaa.cnr.it

For which data product are you filling in this questionnaire?

Answer:
Atmospheric temperature profiles from ground-based microwave radiometer (MWR)

Please provide one or more accessible sources of information that a non-expert user can refer to, to gain an understanding of the measurement technique.

Answer:
EU COST EG-CLIMET Final report – MWR Section:
http://cfa.aquila.infn.it/wiki.eg-climet.org/index.php5/Microwave_radiometer
MWR on Wikipedia (prepared by ITARS fellows, itars.uni-koeln.de):
https://en.wikipedia.org/wiki/Microwave_radiometer

2. Recommended literature

Which literature work would you recommend to understand better the measurement technique and the ***general uncertainty framework*** *within which uncertainties of the data product are constructed. Note that for metrology, the vocabulary list of the VIM (*International Vocabulary of Metrology*), and the uncertainty framework of the GUM (Guide to expression of uncertainty) are important standards. Please provide a complete reference or doi where possible.*

Answer:

Hewison, T. (2006), Profiling Temperature and Humidity by Ground-based Microwave Radiometers, PhD Thesis, University of Reading. Online: http://tim.hewison.org/Thesis.pdf
Küchler, N., D. D. Turner, U. Löhnert, and S. Crewell (2016), Calibrating ground-based microwave radiometers: Uncertainty and drifts, Radio Sci., 51, 311–327, doi:10.1002/2015RS005826.
Maschwitz, G., U. Löhnert, S. Crewell, T. Rose, and D. Turner (2013), Investigation of ground-based microwave radiometer calibration techniques at 530 hPa, Atm. Meas. Tech., 6, 2641–2658, doi:10.5194/amt-6-2641-2013.
Rodgers, C.D. (2000), Inverse Methods for Atmospheric Sounding: Theory and Practice, World Scientific Publishing Co. Ltd. ISBN: 978-981-02-2740-1

More specifically, which literature works (article, ATBD, other…) would you recommend to understand better how uncertainties of this particular data product are conceived? Please provide *a complete reference or doi where possible.*

Answer:

Cadeddu, M. P., Liljegren, J. C., and Turner, D. D. (2013), The Atmospheric radiation measurement (ARM) program network of microwave radiometers: instrumentation, data, and retrievals, Atmos. Meas. Tech., 6, 2359-2372, doi:10.5194/amt-6-2359-2013.

Cimini, D., T. J. Hewison, L. Martin, J. Güldner, C. Gaffard and F. S. Marzano (2006), Temperature and humidity profile retrievals from ground-based microwave radiometers during TUC, Met. Zeitschrift, 15, 1, 45-56, doi: 10.1127/0941-2948/2006/0099.

Cimini D., E. Campos, R. Ware, S. Albers, G. Giuliani, J. Oreamuno, P. Joe, S. Koch, S. Cober, and E. Westwater (2011), Thermodynamic Atmospheric Profiling during the 2010 Winter Olympics Using Ground-based Microwave Radiometry, IEEE Trans. Geosci. Rem. Sens., 49, 12, 4959-4969. doi: 10.1109/TGRS.2011.2154337.

Löhnert, U. and O. Maier (2012), Operational profiling of temperature using ground-based microwave radiometry at Payerne: prospects and challenges, Atmos. Meas. Tech., 5, 1121-1134, doi:10.5194/amt-5-1121-2012.

Maschwitz, G. (2012), Assessment of Ground-Based Microwave Radiometer Calibration to Enable Investigation of Gas Absorption Models. PhD thesis, Universität zu Köln. Online: http://kups.ub.uni-koeln.de/5390/1/DissertationGerritMaschwitz.pdf

Hewison, T. (2007), 1D-VAR retrievals of temperature and humidity profiles from a ground-based microwave radiometer, IEEE Trans. Geosci. Rem. Sens., 45, 7, 2163-2168, doi: 10.1109/TGRS.2007.898091.

Please specify also if the literature source is still up-to-date with the current data product. If not, where can a user find the information on the latest version of the data product and its uncertainties?

Answer:

Most of the current MWR data products do not include uncertainties. Exceptions are the MWR products produced by the ARM Program (Atmospheric Measurement Program, www.arm.gov) and by the HD(CP)^2 project (High Definition Clouds and Precipitation for Climate Prediction, https://hdcp2.zmaw.de). Uncertainties in MWR derived products are usually estimated *ex ante* though simulated analysis (Cadeddu et al., 2013) or *ex post* through validation against collocated radiosonde profiles (Löhnert and Maier, 2012). Dynamical uncertainty estimates have been proposed (Hewison, 2007; Cimini et al., 2011) but have been so far computed for limited datasets (i.e. not operationally and for limited time periods and MWR units).

3. Main measured quantity (measurand)

3.1 Specification of measurand

Specify the main measured quantities (i.e., the measurands) and the associated unit of the data product, along with their field name in the data product

Example measurands with unit: Temperature [K], O3 profile [ppmv], water vapour [ppmv]

Quantity [unit]	Field name

Brightness Temperature [K]	tb
Atmospheric temperature [K]	ta

3.2 Measurement equation

What is the relation between the main measured quantity of the data product and input quantities? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to literature publications).

Answer:
The primary measured quantity is downwelling brightness temperature (tb). Atmospheric temperature (ta) is derived from tb through an inversion method, usually multivariate regression, neural network, or optimal estimation. These methods are described in Cimini et al. (2006).
A brief summary is given below.
The primary observable tb is related to the atmospheric state through the radiative transfer equation, which can be written in its discrete form as:

$$\mathbf{y} = \mathbf{F}(\mathbf{x}) + \boldsymbol{\varepsilon}$$

where **y** is the measurement vector (tb and ancillary data), **x** is the atmospheric state vector (ta in this case), **F** is the operator relating the measurements to the unknown atmospheric state vector, and **ε** is the measurements uncertainty. A general solution is given by optimal estimation (Rodgers, 2000). For the linear case, the solution can be written as:

$$\hat{\mathbf{x}} = \mathbf{x}_\mathrm{b} + [\mathbf{B}^{-1} + \mathbf{K}^\mathrm{T}\mathbf{R}^{-1}\mathbf{K}]^{-1}\mathbf{K}^\mathrm{T}\mathbf{R}^{-1}(\mathbf{y} - \mathbf{K}\mathbf{x}_\mathrm{b})$$

If a priori data set of simultaneous **x** and **y** is available, this may be solved through multivariate linear regression:

$$\hat{\mathbf{x}} = \mathbf{x}_0 + \mathbf{C}_{\mathbf{xy}} \cdot \mathbf{C}_{\mathbf{yy}}{}^{-1}(\mathbf{y} - \mathbf{y}_0)$$

For moderately non-linear problems, the solution is achieved by iteration:

$$\hat{\mathbf{x}}_{i+1} = \hat{\mathbf{x}}_i + \left[\mathbf{B}^{-1} + \mathbf{K}_i^\mathrm{T}\mathbf{R}^{-1}\mathbf{K}_i\right]^{-1} \cdot \left[\mathbf{K}_i^\mathrm{T}\mathbf{R}^{-1}(\mathbf{y} - F(\hat{\mathbf{x}}_i)) - \mathbf{B}^{-1}(\hat{\mathbf{x}}_i - \mathbf{x}_b)\right]$$

where:
y the measurement vector
$\mathbf{y}_0$ the mean measurement vector
x the atmospheric state vector
$\mathbf{x}_b$ the background (a priori) atmospheric state vector
$\mathbf{x}_0$ the mean atmospheric state vector
$\hat{\mathbf{x}}$ the estimated atmospheric state vector
K the Jacobian matrix of the observation vector with respect to the state vector
ε the measurements uncertainty
B the background (a priori) uncertainty covariance matrices
R the measurement uncertainty covariance matrices
$\mathbf{C}_{xy}$ the covariance matrix extracted from a priori data set of simultaneous **x** and **y**
$\mathbf{C}_{yy}$ the autocovariance matrix extracted from a priori data set of **y**

4. Traceability and comparability

4.1 SI or community traceability

Is the measurement quantity traceable, via an unbroken chain of processing steps, to SI units or community accepted standards?

Answer:
No at the present time. Traceability chains are available on www.gaia-clim.eu .

If yes, please provide references to available literature describing the traceability aspects of the measurement.

If no, please describe what aspects of the measurement are not fully traceable and how this aspect is addressed in deriving the data product and its uncertainty.

The following aspects are not fully traceable.

Target emissivity and temperature sensors
The MWR measurement traceability needs to be enforced in the calibration procedure (transfer from raw voltages to tb). This implies the use of certified black-body targets and temperature sensors (measuring the target temperature). Commercial black-body targets have reached a mature state, but the manufacturer's data are usually limited (e.g. 18 GHz is a typical maximum frequency even if the target is used above that frequency). Despite many realizations of microwave brightness temperature standards exist in the form of heated or cooled calibration targets, none are currently maintained as a national standard by a National Measurement Institute (NMI). Metrology applicable to microwave remote sensing radiometry is currently under development, including tb standards. It is expected that SI-traceable tb calibration for black-body targets and transfer standards in the form of calibrated black-body targets will be available in the next few years.
Currently the target emissivity is assumed to be unity within -40 dB (i.e. between 0.9999 and 1.0). The calibration error associated to that uncertainty should be negligible.

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Absorption of radiation by atmospheric gases and hydrometeors is quantitatively modelled while solving the forward problem through the radiative transfer equation. Thus, absorption model uncertainties affect all the retrieval methods based on simulated brightness temperatures. Only retrieval methods based on historical datasets of MWR observations and simultaneous atmospheric soundings are not affected by absorption model uncertainties (e.g. measurement-based regression in Cimini et al., 2006).
A proper characterization of the absorption model contribution to the total uncertainty is lacking. Currently, the absorption model uncertainty is estimated as the difference among existing most common absorption models.

4.2 Comparability

If measurements are taken at multiple sites, are efforts made to ensure sufficiently similar measurement technique approaches to ensure comparability? Please provide links to any supporting materials available such as instrument manuals / network protocols.

Answer:
Protocols to ensure sufficiently similar measurements have been developed by ARM (Cadeddu et al., 2013) and are currently applied for MWR measurements taken at their sites.
Similar efforts are carried out within TOPROF (www.toprof.eu) and previous EU COST actions, e.g. reports from the Joint Calibration Experiments (JCAL 1[1] and 2[2]) and MWRnet[3].

[1] http://tinyurl.com/JCAL1-report-pdf
[2] http://tinyurl.com/JCAL2-report-pdf
[3] http://cetemps.aquila.infn.it/mwrnet/main_files/reports.html

5. Representation of the uncertainty in the data product

5.1 Uncertainty field name(s)

Which field name(s) are used in the data product to hold the uncertainty value(s) associated with the main measured quantities? Note that more than one uncertainty field name can be associated with a single quantity (e.g., one field name for the "uncertainty due to random effects" and one for the "uncertainty due to systematic effects").

Field name of uncertainty	Associated quantity
offset_tb	brightness temperature offset subtracted from measured brightness temperature
tb_bias	systematic calibration uncertainty of brightness temperature, one standard deviation
tb_cov	error covariance matrix of brightness temperature channels
ta_offset	atmospheric temperature offset correction based on brightness temperature offset
ta_err	standard error of air_temperature

5.2 Uncertainty form

In what form is the uncertainty per measurement represented in the data product? For example, is it:

- *A standard uncertainty (i.e., uncertainty expressed as standard deviation)*
- *A 95% coverage interval*
- *A variance-covariance matrix (if so, explain between which quantities the covariance is taken into account)*
- *A probability density function*
- *Other [please specify]*

Answer:
A standard uncertainty (i.e., uncertainty expressed as standard deviation)

6. Uncertainty calculation

6.1 Formula/procedure

What is the formula/procedure by which the uncertainty is calculated? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to one or more equations in the literature).

Answer:
When using regression, the estimated retrieval uncertainty is given as the standard deviation of the residuals ($\delta\mathbf{x} = \hat{\mathbf{x}} - \mathbf{x}_{true}$), i.e. the difference between the estimated ($\hat{\mathbf{x}}$) and the true ($\mathbf{x}_{true}$) atmospheric states for each member of the a priori data set:

$$u(\mathbf{x}) = \mathbf{std}(\delta\mathbf{x}) = \mathbf{std}(\hat{\mathbf{x}} - \mathbf{x}_{true})$$

When using an optimal estimation method, the estimated retrieval uncertainty is given by the diagonal terms of the posterior covariance matrix (same notation as 3.2 above):

$$\mathbf{S}_i = \left[\mathbf{B}^{-1} + \mathbf{K}_i^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{K}_i\right]^{-1}$$
$$u(\mathbf{x}) = \mathbf{diag}(\mathbf{S}_i)$$

Is the uncertainty obtained by:

- *Uncertainty propagation, taking into account the uncertainties of the input quantities,*
- *Probability density function propagation,*
- *Sensitivity analysis: i.e., varying parameters and check the impact on the output quantity,*
- *Or still some other procedure?*

Answer:
For tb, the uncertainty is estimated through sensitivity analysis (Maschwitz, 2012).
For the atmospheric retrieval (in this case the atmospheric temperature ta), the uncertainty is estimated through
- when using regression: the standard deviation of the residuals from the a priori data set;
- when using optimal estimation method: uncertainty propagation (optimal estimation formalism; Rodgers, 2000).

6.2 Level of approximation

In what way is the uncertainty calculation procedure an approximation?

- *Is it based on (as is common practice) a first-order Taylor approximation (see GUM, Eq. (13))*

$$u_c^2(y) = \sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i,x_j) = \sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i,x_j)$$

  which will not be exact if f is nonlinear.

- *Are correlations between input quantities neglected?*
- *Other approximations?*

Answer:
The uncertainty calculation is based on a first-order Taylor approximation.
Correlation between simultaneous measurements at different channels is usually neglected.

If an approximation is involved, do you think the approximation can be a problem, or do you consider it justified?

Answer:
The problem is moderately non-linear (Rodgers, 2000).
Investigation on the covariance matrix of simultaneous measurements at different channels shows small off-diagonal terms.
Thus, the above approximations are considered justified.

7. Uncertainty contributions

7.1 Prior

Is there a prior contribution? If so, is this prior based on measured data, a model, a rough guess, or something else?

Answer:
Atmospheric MWR radiometry is an ill-posed problem and thus prior information is essentials for constraining the solution. Usually prior information comes from either a climatological mean of measured data (e.g. radiosondes) or the output of an atmospheric model (e.g. analysis).
In the first case, the climatological mean, the uncertainty of the prior is estimated as the standard deviation of the measured dataset (e.g. multi-year radiosonde ensemble).
In the other case, the atmospheric model output, the uncertainty of the prior is estimated as the model background error covariance matrix.

7.2 Smoothing error

Is an error source "smoothing error" included in the uncertainty calculation? If so, what do you define as "smoothing error"? Should the averaging kernel of the data product be applied in some way, before the uncertainty can be properly interpreted?

Answer:
The smoothing error is part of the total uncertainty estimated with the optimal estimation method.
The smoothing error is defined as $(\mathbf{A}-\mathbf{I})(\mathbf{x}-\mathbf{x_b})$ whose covariance is $\mathbf{S}_\mathrm{S} = (\mathbf{A}-\mathbf{I})\mathbf{B}(\mathbf{A}-\mathbf{I})^T$ (Rodgers 2000, Section 3), where **A** is the averaging kernel matrix:

$$\mathbf{A}_i = \left[\mathbf{B}^{-1} + \mathbf{K}_i^\mathrm{T}\mathbf{R}^{-1}\mathbf{K}_i\right]^{-1}\mathbf{K}_i^\mathrm{T}\mathbf{R}^{-1}\mathbf{K}_i$$

Thus, if the smoothing error needs to be separated from the total uncertainty, the averaging kernel matrix **A** is needed. This is currently not provided in the data files. However, the averaging kernel matrix may be provided in the future, either computed from the optimal estimation formalism above or through a brute force approach (Löhnert and Maier, 2012).

7.3 Noise

Is there a noise contribution? If so, what do you define as "noise"? (E.g., for MOPITT, one considers an instrumental noise, but also a "geophysical noise" (Deeter, 2013).)

Answer:
Instrumental noise is considered as the random uncertainty affecting tb observations (i.e. radiometric noise).
Geophysical noise in this context may be interpreted to be the "representativeness error", i.e. the uncertainty deriving from the background spatial/temporal variability at the place/time of its use. This contribution represents the uncertainty in the generalized interpolation from background to observations (Hewison, 2007) and thus it is time variant and depends on atmospheric conditions. This contribution is currently not considered. It may be considered in the future as a contribution to the background or measurement covariance matrices, depending on its used definition.

7.4 Random and systematic contributions

Do you consider explicitly separately "random", "structured random" and "systematic" contributions? If so, how do you define each of these in your calculation?

Answer:
Random uncertainty for tb and ta are considered. Systematic calibration uncertainty for tb is considered. Systematic uncertainty of atmospheric absorption model is currently neglected (it may be considered in the future).

7.5 Input quantities / other parameters

If the main measured quantities of the data product depend on input quantities, how do the final uncertainties depend on uncertainties of these input quantities? Please provide a list with input quantities of which the uncertainties:

1. *Are taken into account.*
2. *Could be important, but are not taken into account. For example, because their consideration would be technically difficult, or it is not clear how to estimate the associated uncertainty.*
3. *Are not taken into account, as they can be demonstrated to be negligible.*

If this list is already available somewhere in a literature source, you can simply refer to it.

Input quantity/other parameter	associated uncertainty or "important but ignored" or "negligible"	Extra info (e.g., random, systematic)
prior	**B** (see equations above)	random

tb	tb_cov, tb_bias	random, systematic
forward model	Potentially important but ignored	systematic (most probably)
target emissivity	Negligible (if the claimed specification for target reflectivity (-40dB) are verified)	systematic

7.6 Uncertainty due to model error

Do you consider explicitly an uncertainty contribution due to the fact that the model is not perfect? Such uncertainty can be revealed e.g., by comparing results of several retrieval models.

Answer:
Absorption model uncertainty shall be considered. This is currently estimated by differences among most used existing absorption models. A proper estimate should consider the sensitivity to forward model parameter uncertainty.

8. Correlations/covariances

8.1 Presence in data product

Do you provide correlations or covariances within your data product, directly relevant to the main measured quantity? If so, between which quantities?

Answer:
The covariance between measurements at different channels is provided in the data files (tb_cov). When using optimal estimation method, the diagonal terms of the posterior covariance matrix are provided in the data files (ta_err). If required, the full posterior covariance matrix could be provided.

Please state in the table below which of the quantities are reported and/or included in the total error. Please use either yes, no or N/A for the first 2 columns and a short explanation in the 3rd. column. Add other quantities as relevant.

Quantity	Explicitly reported	Included in total error	Where reported / name given / comments
measurement noise covariance matrix	Yes	Yes	This is **R** in 3.2 and tb_cov in 5.1
a priori covariance matrix	No	Yes	This is **B** in 3.2
a posteriori covariance matrix	No	Yes	This is **S** in 6.1

8.2 Auto-correlation

Suppose a user has to average several measured values of your data product. E.g., they want the mean column, 100 km around the observation site, within one month. Can you give a recommendation how they can obtain the uncertainty of this mean column, starting from the uncertainties provided for the individual columns?

Answer:
The uncertainty of the average product may be estimated from the standard deviation of the averaged sample. This unlikely happens to be smaller than the average of the individual uncertainties, but in such a case I would suggest to take the latter as the uncertainty estimate.

8.3 Correlation between main measured quantity and other quantities

Do you provide any correlation info between the main measured quantity (e.g., an ozone profile) and other quantities (e.g., a temperature profile)?

Answer:
No.

9. Bias handling introduced during processing

Biases can, at least in theory, be introduced during processing. For example by nonlinear measurement equations in combination with large uncertainties on the input quantities. Is this something you try to correct for, or report, or deal with in some other way? Or do you think this will be negligible?

Answer:
Biases are introduced by calibration and forward model uncertainties. Bias correction on tb is provided for some sites (offset_tb). The propagation of this bias onto retrieved atmospheric temperature may also be provided (ta_offset).

10. Other remarks on data product uncertainty

Please put here any other information about the data product uncertainty that you think is important.

Since MWRnet is an unfunded, bottom-up network, different levels of characterization are currently available among members. A common processing would significantly reduce this heterogeneity; activities towards this goal are ongoing but may not be totally implemented within the available dataset.

Annex G

GAIA-CLIM questionnaire about uncertainty in data products

MWR – Total water vapour content (TWVC)

Table of Contents

1. Identification of respondent and of data product

What are your contact details?

Answer:
Domenico Cimini
National Research Council of Italy – Institute of Methodologies for Environmental Monitoring (CNR-IMAA)
C.da S.Loja, 85050, Tito Scalo, Potenza
Phone: +39/3311706062
E-mail: domenico.cimini@imaa.cnr.it

For which data product are you filling in this questionnaire?

Answer:
Atmospheric total water vapour content (TWVC) from ground-based microwave radiometer (MWR)

Please provide one or more accessible sources of information that a non-expert user can refer to, to gain an understanding of the measurement technique.

Answer:
EU COST EG-CLIMET Final report – MWR Section:
http://cfa.aquila.infn.it/wiki.eg-climet.org/index.php5/Microwave_radiometer
MWR on Wikipedia (prepared by ITARS fellows, itars.uni-koeln.de):
https://en.wikipedia.org/wiki/Microwave_radiometer
ARM MWR Retrievals Value-Added Product (MWRRET VAP):
https://www.arm.gov/data/vaps/mwrret

2. Recommended literature

*Which literature work would you recommend to understand better the measurement technique and the **general uncertainty framework** within which uncertainties of the data product are constructed. Note that for metrology, the vocabulary list of the VIM (*International Vocabulary of Metrology*), and the uncertainty framework of the GUM (Guide to expression of uncertainty) are important standards. Please provide a complete reference or doi where possible.*

Answer:
Han, Y. and E. R. Westwater (2000), Analysis and Improvement of Tipping Calibration for Ground-based Microwave Radiometers. IEEE Trans. Geosci. Remote Sens., 38(3), 1260–127, doi: 10.1109/36.843018.

Küchler, N., D. D. Turner, U. Löhnert, and S. Crewell (2016), Calibrating ground-based microwave radiometers: Uncertainty and drifts, Radio Sci., 51, 311–327, doi:10.1002/2015RS005826.

Maschwitz, G., U. Löhnert, S. Crewell, T. Rose, and D. Turner (2013), Investigation of ground-based microwave radiometer calibration techniques at 530 hPa, Atm. Meas. Tech., 6, 2641–2658, doi:10.5194/amt-6-2641-2013.

Rodgers, C.D. (2000), Inverse Methods for Atmospheric Sounding: Theory and Practice, World Scientific Publishing Co. Ltd. ISBN: 978-981-02-2740-1

More specifically, which literature works (article, ATBD, other…) would you recommend to understand better how uncertainties of this particular data product are conceived? Please provide *a complete reference or doi where possible.*

Answer:

Cadeddu, M. P., Liljegren, J. C., and Turner, D. D. (2013), The Atmospheric radiation measurement (ARM) program network of microwave radiometers: instrumentation, data, and retrievals, Atmos. Meas. Tech., 6, 2359-2372, doi:10.5194/amt-6-2359-2013.

Cimini, D., T. J. Hewison, L. Martin, J. Güldner, C. Gaffard and F. S. Marzano (2006), Temperature and humidity profile retrievals from ground-based microwave radiometers during TUC, Met. Zeitschrift, 15, 1, 45-56, doi: 10.1127/0941-2948/2006/0099.

Maschwitz, G. (2012), Assessment of Ground-Based Microwave Radiometer Calibration to Enable Investigation of Gas Absorption Models. PhD thesis, Universität zu Köln. Online: http://kups.ub.uni-koeln.de/5390/1/DissertationGerritMaschwitz.pdf

Turner, D.D., S.A. Clough, J.C. Liljegren, E.E. Clothiaux, K. Cady-Pereira, and K.L. Gaustad, 2007: Retrieving liquid water path and precipitable water vapor from Atmospheric Radiation Measurement (ARM) microwave radiometers. IEEE Trans. Geosci. Remote Sens., 45, 3680-3690, doi:10.1109/TGRS.2007.903703.

Please specify also if the literature source is still up-to-date with the current data product. If not, where can a user find the information on the latest version of the data product and its uncertainties?

Answer:

The literature sources above are still up-to-date. Uncertainties in MWR products are provided by the ARM Program (Atmospheric Measurement Program, www.arm.gov) and by the HD(CP)[2] project (High Definition Clouds and Precipitation for Climate Prediction, https://hdcp2.zmaw.de). Uncertainties in MWR derived products are usually estimated *ex ante* through simulated analysis and/or *ex post* through validation against collocated radiosonde profiles (Cadeddu et al., 2013). Dynamical uncertainty estimates are provided with the ARM MWR Retrievals (MWRRET) Value-Added Product (VAP) (Turner et al., 2007; Cadeddu et al., 2013).

3. Main measured quantity (measurand)

3.1 Specification of measurand

Specify the main measured quantities (i.e., the measurands) and the associated unit of the data product, along with their field name in the data product

Example measurands with unit: Temperature [K], O3 profile [ppmv], water vapour [ppmv]

Quantity [unit]	Field name
Brightness Temperature [K]	tb
Total water vapour content [kg m-2]	prw

3.2 Measurement equation

What is the relation between the main measured quantity of the data product and input quantities? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to literature publications).

Answer:
The primary measured quantity is downwelling brightness temperature (tb). Atmospheric total water vapour content (prw) is derived from tb through an inversion method, usually multivariate regression, neural network, or optimal estimation. These methods are described in Cimini et al. (2006). A brief summary is given below.
The primary observable tb is related to the atmospheric state through the radiative transfer equation, which can be written in its discrete form as:

$$\mathbf{y} = \mathbf{F}(\mathbf{x}) + \boldsymbol{\varepsilon}$$

where **y** is the measurement vector (tb and ancillary data), **x** is the atmospheric state vector (ta in this case), **F** is the operator relating the measurements to the unknown atmospheric state vector, and **ε** is the measurements uncertainty. A general solution is given by optimal estimation (Rodgers, 2000). Since the relation between TWVC and atmospheric opacity is nearly linear, the optimal estimation solution is given by:

$$\hat{\mathbf{x}} = \mathbf{x}_b + [\mathbf{B}^{-1} + \mathbf{K}^T\mathbf{R}^{-1}\mathbf{K}]^{-1}\mathbf{K}^T\mathbf{R}^{-1}(\mathbf{y} - \mathbf{K}\mathbf{x}_b)$$

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Is the uncertainty obtained by:

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Answer:
For tb, the uncertainty is estimated through sensitivity analysis (Maschwitz, 2012).
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In what way is the uncertainty calculation procedure an approximation?

- *Is it based on (as is common practice) a first-order Taylor approximation (see GUM, Eq. (13))*

$$u_c^2(y) = \sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i,x_j) = \sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i,x_j)$$

  which will not be exact if f is nonlinear.

- *Are correlations between input quantities neglected?*
- *Other approximations?*

Answer:
The uncertainty calculation is based on a first-order Taylor approximation.
Correlation between simultaneous measurements at different channels is usually neglected.

If an approximation is involved, do you think the approximation can be a problem, or do you consider it justified?

Answer:
The problem is nearly linear (Turner et al., 2007).
Investigation on the covariance matrix of simultaneous measurements at different channels shows small off-diagonal terms.
Thus, the above approximations are considered justified.

7. Uncertainty contributions

7.1 Prior

Is there a prior contribution? If so, is this prior based on measured data, a model, a rough guess, or something else?

Answer:
Atmospheric MWR radiometry is an ill-posed problem and thus prior information is essentials for constraining the solution. Prior information comes from either a climatological mean of measured data, or the output of an atmospheric model (e.g. analysis), or time interpolation of the closest measured data (e.g. radiosondes).
In the first case, the climatological mean, the uncertainty of the prior is estimated as the standard deviation of the measured dataset (e.g. multi-year radiosonde ensemble).
In the second case, the atmospheric model output, the uncertainty of the prior is estimated as the model background error covariance matrix.
In the latter case, the time interpolation, zero uncertainty is assumed on the temperature and the humidity profiles (though the latter is scaled by a height-independent factor to match the MWR TWVC), while the uncertainty of the TWVC prior is set to a very large value (e.g. 20 kg/m^2) (Turner et al., 2007).

7.2 Smoothing error

Is an error source "smoothing error" included in the uncertainty calculation? If so, what do you define as "smoothing error"? Should the averaging kernel of the data product be applied in some way, before the uncertainty can be properly interpreted?

Answer:

The smoothing error is part of the total uncertainty estimated with the optimal estimation method. The smoothing error is defined as $(\mathbf{A}-\mathbf{I})(\mathbf{x}-\mathbf{x_b})$ whose covariance is $\mathbf{S}_S = (\mathbf{A}-\mathbf{I})\mathbf{B}(\mathbf{A}-\mathbf{I})^T$ (Rodgers 2000, Section 3), where **A** is the averaging kernel matrix:

$$\mathbf{A}_i = \left[\mathbf{B}^{-1} + \mathbf{K}_i^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{K}_i\right]^{-1}\mathbf{K}_i^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{K}_i$$

For vertically-integrated total column retrievals such as TWVC, the averaging kernels are also vertically integrated. Thus, if the smoothing error needs to be separated from the total uncertainty, the averaging kernel matrix **A** is needed. This is currently not provided in the data files. This is considered as non-critical as MWR sensitivity to water vapour is only weakly height-dependent.

7.3 Noise

Is there a noise contribution? If so, what do you define as “noise”? (E.g., for MOPITT, one considers an instrumental noise, but also a “geophysical noise” (Deeter, 2013).)

Answer:
Instrumental noise is considered as the random uncertainty affecting tb observations (i.e. radiometric noise).
The contribution of geophysical noise is not considered, as this concept does not seem to apply in the context of TWVC retrievals.

7.4 Random and systematic contributions

Do you consider explicitly separately “random”, “structured random” and “systematic” contributions? If so, how do you define each of these in your calculation?

Answer:
Random uncertainty for tb and pwr are considered. Systematic calibration uncertainty for tb is considered. Systematic uncertainty of atmospheric absorption model is currently neglected (it may be considered in the future).

7.5 Input quantities / other parameters

If the main measured quantities of the data product depend on input quantities, how do the final uncertainties depend on uncertainties of these input quantities? Please provide a list with input quantities of which the uncertainties:

1. *Are taken into account.*
2. *Could be important, but are not taken into account. For example, because their consideration would be technically difficult, or it is not clear how to estimate the associated uncertainty.*
3. *Are not taken into account, as they can be demonstrated to be negligible.*

If this list is already available somewhere in a literature source, you can simply refer to it.

Input quantity/other parameter	associated uncertainty or “important but ignored” or “negligible”	Extra info (e.g., random, systematic)
prior	**B** (see equations above)	random
tb	tb_cov, tb_bias	random, systematic
forward model	Potentially important but ignored	systematic (most probably)
target emissivity	Negligible (if the claimed specification for target reflectivity (-40dB) are verified)	systematic

7.6 Uncertainty due to model error

Do you consider explicitly an uncertainty contribution due to the fact that the model is not perfect? Such uncertainty can be revealed e.g., by comparing results of several retrieval models.

Answer:
Absorption model uncertainty shall be considered. This is currently estimated by differences among most used existing absorption models. A proper estimate should consider the sensitivity to forward model parameter uncertainty.

8. Correlations/covariances

8.1 Presence in data product

Do you provide correlations or covariances within your data product, directly relevant to the main measured quantity? If so, between which quantities?

Answer:
The covariance between measurements at different channels is provided in the data files (tb_cov).

Please state in the table below which of the quantities are reported and/or included in the total error. Please use either yes, no or N/A for the first 2 columns and a short explanation in the 3rd. column. Add other quantities as relevant.

Quantity	Explicitly reported	Included in total error	Where reported / name given / comments
measurement noise covariance matrix	Yes	Yes	This is **R** in 3.2 and tb_cov in 5.1
a priori covariance matrix	No	Yes	This is **B** in 3.2

8.2 Auto-correlation

Suppose a user has to average several measured values of your data product. E.g., they want the mean column, 100 km around the observation site, within one month. Can you give a recommendation how they can obtain the uncertainty of this mean column, starting from the uncertainties provided for the individual columns?

Answer:
The uncertainty of the average product may be estimated from the standard deviation of the averaged sample. This unlikely happens to be smaller than the average of the individual uncertainties, but in such a case I would suggest to take the latter as the uncertainty estimate.

8.3 Correlation between main measured quantity and other quantities

Do you provide any correlation info between the main measured quantity (e.g., an ozone profile) and other quantities (e.g., a temperature profile)?

Answer: No.

9. Bias handling introduced during processing

Biases can, at least in theory, be introduced during processing. For example by nonlinear measurement equations in combination with large uncertainties on the input quantities. Is this something you try to correct for, or report, or deal with in some other way? Or do you think this will be negligible?

Answer:
Biases are introduced by calibration and forward model uncertainties. Bias correction on tb is provided for some sites (offset_tb). The propagation of this bias onto retrieved TWVC may also be provided (prw_offset).

10. Other remarks on data product uncertainty

Please put here any other information about the data product uncertainty that you think is important.

Since MWRnet is an unfunded, bottom-up network, different levels of characterization are currently available among members. A common processing would significantly reduce this heterogeneity; activities towards this goal are ongoing but may not be totally implemented within the available dataset.

Annex H

GAIA-CLIM questionnaire about uncertainty in data products

MWR – Total liquid water content (TLWC)

Table of Contents

1. Identification of respondent and of data product

What are your contact details?

Answer:

Domenico Cimini
National Research Council of Italy – Institute of Methodologies for Environmental Monitoring (CNR-IMAA)
C.da S.Loja, 85050, Tito Scalo, Potenza
Phone: +39/3311706062
E-mail: domenico.cimini@imaa.cnr.it

For which data product are you filling in this questionnaire?

Answer:
Atmospheric total liquid water content (TLWC) from ground-based microwave radiometer (MWR)

Please provide one or more accessible sources of information that a non-expert user can refer to, to gain an understanding of the measurement technique.

Answer:
EU COST EG-CLIMET Final report – MWR Section:
http://cfa.aquila.infn.it/wiki.eg-climet.org/index.php5/Microwave_radiometer
MWR on Wikipedia (prepared by ITARS fellows, itars.uni-koeln.de):
https://en.wikipedia.org/wiki/Microwave_radiometer
ARM MWR Retrievals Value-Added Product (MWRRET VAP):
https://www.arm.gov/data/vaps/mwrret

2. Recommended literature

*Which literature work would you recommend to understand better the measurement technique and the **general uncertainty framework** within which uncertainties of the data product are constructed. Note that for metrology, the vocabulary list of the VIM (*International Vocabulary of Metrology*), and the uncertainty framework of the GUM (Guide to expression of uncertainty) are important standards. Please provide a complete reference or doi where possible.*

Answer:

Han, Y. and E. R. Westwater (2000), Analysis and Improvement of Tipping Calibration for Ground-based Microwave Radiometers. IEEE Trans. Geosci. Remote Sens., 38(3), 1260–127, doi: 10.1109/36.843018.

Küchler, N., D. D. Turner, U. Löhnert, and S. Crewell (2016), Calibrating ground-based microwave radiometers: Uncertainty and drifts, Radio Sci., 51, 311–327, doi:10.1002/2015RS005826.

Maschwitz, G., U. Löhnert, S. Crewell, T. Rose, and D. Turner (2013), Investigation of ground-based microwave radiometer calibration techniques at 530 hPa, Atm. Meas. Tech., 6, 2641–2658, doi:10.5194/amt-6-2641-2013.

Rodgers, C.D. (2000), Inverse Methods for Atmospheric Sounding: Theory and Practice, World Scientific Publishing Co. Ltd. ISBN: 978-981-02-2740-1

More specifically, which literature works (article, ATBD, other…) would you recommend to understand better how uncertainties of this particular data product are conceived? Please provide *a complete reference or doi where possible.*

Answer:

Cadeddu, M. P., Liljegren, J. C., and Turner, D. D. (2013), The Atmospheric radiation measurement (ARM) program network of microwave radiometers: instrumentation, data, and retrievals, Atmos. Meas. Tech., 6, 2359-2372, doi:10.5194/amt-6-2359-2013.

Cimini, D., T. J. Hewison, L. Martin, J. Güldner, C. Gaffard and F. S. Marzano (2006), Temperature and humidity profile retrievals from ground-based microwave radiometers during TUC, Met. Zeitschrift, 15, 1, 45-56, doi: 10.1127/0941-2948/2006/0099.

Crewell S. and U. Löhnert, 2003: Accuracy of cloud liquid water path from ground-based microwave radiometry, 2. Sensor accuracy and synergy. Radio Sci., 38, 8042, doi: 10.1029/2002RS002634.

Löhnert U. and S. Crewell, 2003: Accuracy of cloud liquid water path from groud-based microwave radiometry. Part I. Dependency on cloud model statistics. Radio Sci. 38, 8041, doi:10.1029/202RS002654.

Maschwitz, G. (2012), Assessment of Ground-Based Microwave Radiometer Calibration to Enable Investigation of Gas Absorption Models. PhD thesis, Universität zu Köln. Online: http://kups.ub.uni-koeln.de/5390/1/DissertationGerritMaschwitz.pdf

Turner, D.D., S.A. Clough, J.C. Liljegren, E.E. Clothiaux, K. Cady-Pereira, and K.L. Gaustad, 2007: Retrieving liquid water path and precipitable water vapor from Atmospheric Radiation Measurement (ARM) microwave radiometers. IEEE Trans. Geosci. Remote Sens., 45, 3680-3690, doi:10.1109/TGRS.2007.903703.

Please specify also if the literature source is still up-to-date with the current data product. If not, where can a user find the information on the latest version of the data product and its uncertainties?

Answer:

The literature sources above are still up-to-date. Uncertainties in MWR products are provided by the ARM Program (Atmospheric Measurement Program, www.arm.gov) and by the $HD(CP)^2$ project (High Definition Clouds and Precipitation for Climate Prediction, https://hdcp2.zmaw.de). Uncertainties in MWR derived products are usually estimated *ex ante* through simulated analysis and/or *ex post* through validation against collocated radiosonde profiles (Cadeddu et al., 2013). Dynamical uncertainty estimates are provided with the ARM MWR Retrievals (MWRRET) Value-Added Product (VAP) (Turner et al., 2007; Cadeddu et al., 2013).

3. Main measured quantity (measurand)

3.1 Specification of measurand

Specify the main measured quantities (i.e., the measurands) and the associated unit of the data product, along with their field name in the data product

Example measurands with unit: Temperature [K], O3 profile [ppmv], water vapour [ppmv]

Quantity [unit]	Field name
Brightness Temperature [K]	tb
Total liquid water content [kg m-2]	clwvi

3.2 Measurement equation

What is the relation between the main measured quantity of the data product and input quantities? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to literature publications).

Answer:
The primary measured quantity is downwelling brightness temperature (tb). Atmospheric total liquid water content (clwvi) is derived from tb through an inversion method, usually multivariate regression, neural network, or optimal estimation. These methods are described in Cimini et al. (2006). A brief summary is given below.
The primary observable tb is related to the atmospheric state through the radiative transfer equation, which can be written in its discrete form as:

$$\mathbf{y} = \mathbf{F}(\mathbf{x}) + \boldsymbol{\varepsilon}$$

where **y** is the measurement vector (tb and ancillary data), **x** is the atmospheric state vector (ta in this case), **F** is the operator relating the measurements to the unknown atmospheric state vector, and **ε** is the measurements uncertainty. A general solution is given by optimal estimation (Rodgers, 2000). Since the relation between TWVC and atmospheric opacity is nearly linear, the optimal estimation solution is given by:

$$\hat{\mathbf{x}} = \mathbf{x}_\mathrm{b} + [\mathbf{B}^{-1} + \mathbf{K}^\mathrm{T}\mathbf{R}^{-1}\mathbf{K}]^{-1}\mathbf{K}^\mathrm{T}\mathbf{R}^{-1}(\mathbf{y} - \mathbf{K}\mathbf{x}_\mathrm{b})$$

If a priori data set of simultaneous **x** and **y** is available, this may be solved through multivariate linear regression:

$$\hat{\mathbf{x}} = \mathbf{x}_0 + \mathbf{C}_\mathbf{xy} \cdot \mathbf{C}_\mathbf{yy}^{-1}(\mathbf{y} - \mathbf{y}_0)$$

where:
y the measurement vector
$\mathbf{y}_0$ the mean measurement vector
x the atmospheric state vector
$\mathbf{x}_b$ the background (a priori) atmospheric state vector
$\mathbf{x}_0$ the mean atmospheric state vector
$\hat{\mathbf{x}}$ the estimated atmospheric state vector
K the Jacobian matrix of the observation vector with respect to the state vector
ε the measurements uncertainty
B the background (a priori) uncertainty covariance matrices
R the measurement uncertainty covariance matrices
$\mathbf{C}_{xy}$ the covariance matrix extracted from a priori data set of simultaneous **x** and **y**

$\mathbf{C_{yy}}$ the autocovariance matrix extracted from a priori data set of $\mathbf{y}$

4. Traceability and comparability

4.1 SI or community traceability

Is the measurement quantity traceable, via an unbroken chain of processing steps, to SI units or community accepted standards?

Answer:
No at the present time. Traceability chains are available on www.gaia-clim.eu .

If yes, please provide references to available literature describing the traceability aspects of the measurement.

If no, please describe what aspects of the measurement are not fully traceable and how this aspect is addressed in deriving the data product and its uncertainty.

The following aspects are not fully traceable.

Target emissivity and temperature sensors
The MWR measurement traceability needs to be enforced in the calibration procedure (transfer from raw voltages to tb). This implies the use of certified black-body targets and temperature sensors (measuring the target temperature). Commercial black-body targets have reached a mature state, but the manufacturer's data are usually limited (e.g. 18 GHz is a typical maximum frequency even if the target is used above that frequency). Despite many realizations of microwave brightness temperature standards exist in the form of heated or cooled calibration targets, none are currently maintained as a national standard by a National Measurement Institute (NMI). Metrology applicable to microwave remote sensing radiometry is currently under development, including tb standards. It is expected that SI-traceable tb calibration for black-body targets and transfer standards in the form of calibrated black-body targets will be available in the next few years.
Currently the target emissivity is assumed to be unity within -40 dB (i.e. between 0.9999 and 1.0). The calibration error associated to that uncertainty should be negligible.

Absorption model
Absorption of radiation by atmospheric gases and hydrometeors is quantitatively modelled while solving the forward problem through the radiative transfer equation. Thus, absorption model uncertainties affect all the retrieval methods based on simulated brightness temperatures. Only retrieval methods based on historical datasets of MWR observations and simultaneous atmospheric soundings are not affected by absorption model uncertainties (e.g. measurement-based regression in Cimini et al., 2006).
A proper characterization of the absorption model contribution to the total uncertainty is lacking. Currently, the absorption model uncertainty is estimated as the difference among existing most common absorption models.

4.2 Comparability

If measurements are taken at multiple sites, are efforts made to ensure sufficiently similar measurement technique approaches to ensure comparability? Please provide links to any supporting materials available such as instrument manuals / network protocols.

Answer:
Protocols to ensure sufficiently similar measurements have been developed by ARM (Cadeddu et al., 2013) and are currently applied for MWR measurements taken at their sites.
Similar efforts are carried out within TOPROF (www.toprof.eu) and previous EU COST actions, e.g. reports from the Joint Calibration Experiments (JCAL 1[1] and 2[2]) and MWRnet[3].

[1] http://tinyurl.com/JCAL1-report-pdf
[2] http://tinyurl.com/JCAL2-report-pdf
[3] http://cetemps.aquila.infn.it/mwrnet/main_files/reports.html

5. Representation of the uncertainty in the data product

5.1 Uncertainty field name(s)

Which field name(s) are used in the data product to hold the uncertainty value(s) associated with the main measured quantities? Note that more than one uncertainty field name can be associated with a single quantity (e.g., one field name for the "uncertainty due to random effects" and one for the "uncertainty due to systematic effects").

Field name of uncertainty	Associated quantity
offset_tb	brightness temperature offset subtracted from measured brightness temperature
tb_bias	systematic calibration uncertainty of brightness temperature, one standard deviation
tb_cov	error covariance matrix of brightness temperature channels
clwvi_offset	TLWC offset correction based on brightness temperature offset
clwvi_err	standard error of TLWC

5.2 Uncertainty form

In what form is the uncertainty per measurement represented in the data product? For example, is it:

- *A standard uncertainty (i.e., uncertainty expressed as standard deviation)*
- *A 95% coverage interval*
- *A variance-covariance matrix (if so, explain between which quantities the covariance is taken into account)*
- *A probability density function*
- *Other [please specify]*

Answer:
A standard uncertainty (i.e., uncertainty expressed as standard deviation)

6. Uncertainty calculation

6.1 Formula/procedure

What is the formula/procedure by which the uncertainty is calculated? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to one or more equations in the literature).

Answer:
When using regression, the estimated retrieval uncertainty is given as the standard deviation of the residuals ($\delta\mathbf{x} = \hat{\mathbf{x}} - \mathbf{x}_{true}$), i.e. the difference between the estimated ($\hat{\mathbf{x}}$) and the true ($\mathbf{x}_{true}$) atmospheric states for each member of the a priori data set:

$$u(\mathbf{x}) = \mathbf{std}(\delta\mathbf{x}) = \mathbf{std}(\hat{\mathbf{x}} - \mathbf{x}_{true})$$

When using an optimal estimation method, the estimated retrieval uncertainty is given by the diagonal terms of the posterior covariance matrix (same notation as 3.2 above):

$$\mathbf{S}_i = \left[\mathbf{B}^{-1} + \mathbf{K}_i^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{K}_i\right]^{-1}$$
$$u(\mathbf{x}) = \mathbf{diag}(\mathbf{S}_i)$$

Is the uncertainty obtained by:

- *Uncertainty propagation, taking into account the uncertainties of the input quantities,*
- *Probability density function propagation,*
- *Sensitivity analysis: i.e., varying parameters and check the impact on the output quantity,*
- *Or still some other procedure?*

Answer:
For tb, the uncertainty is estimated through sensitivity analysis (Maschwitz, 2012).
For the atmospheric retrieval (in this case the total liquid water content), the uncertainty is estimated through
- when using regression: the standard deviation of the residuals from the a priori data set;
- when using optimal estimation method: uncertainty propagation (optimal estimation formalism; Rodgers, 2000).

6.2 Level of approximation

In what way is the uncertainty calculation procedure an approximation?

- *Is it based on (as is common practice) a first-order Taylor approximation (see GUM, Eq. (13))*

$$u_c^2(y) = \sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i, x_j) = \sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i, x_j)$$

which will not be exact if f is nonlinear.

- *Are correlations between input quantities neglected?*
- *Other approximations?*

Answer:
The uncertainty calculation is based on a first-order Taylor approximation.
Correlation between simultaneous measurements at different channels is usually neglected.

If an approximation is involved, do you think the approximation can be a problem, or do you consider it justified?

Answer:
The problem is nearly linear (Turner et al., 2007).
Investigation on the covariance matrix of simultaneous measurements at different channels shows small off-diagonal terms.
Thus, the above approximations are considered justified.

7. Uncertainty contributions

7.1 Prior

Is there a prior contribution? If so, is this prior based on measured data, a model, a rough guess, or something else?

Answer:
Atmospheric MWR radiometry is an ill-posed problem and thus prior information is essentials for constraining the solution. Prior information comes from either a climatological mean of measured data, or the output of an atmospheric model (e.g. analysis), or time interpolation of the closest measured data (e.g. radiosondes).
In the first case, the climatological mean, the uncertainty of the prior is estimated as the standard deviation of the measured dataset (e.g. multi-year radiosonde ensemble).
In the second case, the atmospheric model output, the uncertainty of the prior is estimated as the model background error covariance matrix.
In the latter case, the time interpolation, zero uncertainty is assumed on the temperature and the humidity profiles (though the latter is scaled by a height-independent factor to match the MWR TWVC), while the uncertainty of the TLWC prior is set to a very large value (e.g. 250 g/m^2) (Turner et al., 2007).

7.2 Smoothing error

Is an error source "smoothing error" included in the uncertainty calculation? If so, what do you define as "smoothing error"? Should the averaging kernel of the data product be applied in some way, before the uncertainty can be properly interpreted?

Answer:
The smoothing error is part of the total uncertainty estimated with the optimal estimation method. The smoothing error is defined as $(\mathbf{A}-\mathbf{I})(\mathbf{x}-\mathbf{x_b})$ whose covariance is $\mathbf{S}_S = (\mathbf{A}-\mathbf{I})\mathbf{B}(\mathbf{A}-\mathbf{I})^T$ (Rodgers 2000, Section 3), where **A** is the averaging kernel matrix:

$$\mathbf{A}_i = \left[\mathbf{B}^{-1} + \mathbf{K}_i^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{K}_i\right]^{-1}\mathbf{K}_i^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{K}_i$$

For vertically-integrated total column retrievals such as TLWC, the averaging kernels are also vertically integrated. Thus, if the smoothing error needs to be separated from the total uncertainty, the averaging kernel matrix **A** is needed. This is currently not provided in the data files. This is considered as non-critical as MWR sensitivity to liquid water is only weakly height-dependent.

7.3 Noise

Is there a noise contribution? If so, what do you define as “noise”? (E.g., for MOPITT, one considers an instrumental noise, but also a “geophysical noise” (Deeter, 2013).)

Answer:
Instrumental noise is considered as the random uncertainty affecting tb observations (i.e. radiometric noise).
The contribution of geophysical noise is not considered, as this concept does not seem to apply in the context of TLWC retrievals.

7.4 Random and systematic contributions

Do you consider explicitly separately “random”, “structured random” and “systematic” contributions? If so, how do you define each of these in your calculation?

Answer:
Random uncertainty for tb and clwvi are considered. Systematic calibration uncertainty for tb is considered. Systematic uncertainty of atmospheric absorption model is currently neglected (it may be considered in the future).

7.5 Input quantities / other parameters

If the main measured quantities of the data product depend on input quantities, how do the final uncertainties depend on uncertainties of these input quantities? Please provide a list with input quantities of which the uncertainties:

1. *Are taken into account.*
2. *Could be important, but are not taken into account. For example, because their consideration would be technically difficult, or it is not clear how to estimate the associated uncertainty.*
3. *Are not taken into account, as they can be demonstrated to be negligible.*

If this list is already available somewhere in a literature source, you can simply refer to it.

Input quantity/other parameter	associated uncertainty or "important but ignored" or "negligible"	Extra info (e.g., random, systematic)
prior	**B** (see equations above)	random
tb	tb_cov, tb_bias	random, systematic
forward model	Potentially important but ignored	systematic (most probably)
target emissivity	Negligible (if the claimed specification for target reflectivity (-40dB) are verified)	systematic

7.6 Uncertainty due to model error

Do you consider explicitly an uncertainty contribution due to the fact that the model is not perfect? Such uncertainty can be revealed e.g., by comparing results of several retrieval models.

Answer:
Absorption model uncertainty shall be considered. This is currently estimated by differences among most used existing absorption models. A proper estimate should consider the sensitivity to forward model parameter uncertainty.

8. Correlations/covariances

8.1 Presence in data product

Do you provide correlations or covariances within your data product, directly relevant to the main measured quantity? If so, between which quantities?

Answer:
The covariance between measurements at different channels is provided in the data files (tb_cov).

Please state in the table below which of the quantities are reported and/or included in the total error. Please use either yes, no or N/A for the first 2 columns and a short explanation in the 3rd. column. Add other quantities as relevant.

Quantity	Explicitly reported	Included in total error	Where reported / name given / comments
measurement noise covariance matrix	Yes	Yes	This is **R** in 3.2 and tb_cov in 5.1
a priori covariance matrix	No	Yes	This is **B** in 3.2

8.2 Auto-correlation

Suppose a user has to average several measured values of your data product. E.g., they want the mean column, 100 km around the observation site, within one month. Can you give a recommendation how they can obtain the uncertainty of this mean column, starting from the uncertainties provided for the individual columns?

Answer:
The uncertainty of the average product may be estimated from the standard deviation of the averaged sample. This unlikely happens to be smaller than the average of the individual uncertainties, but in such a case I would suggest to take the latter as the uncertainty estimate.

8.3 Correlation between main measured quantity and other quantities

Do you provide any correlation info between the main measured quantity (e.g., an ozone profile) and other quantities (e.g., a temperature profile)?

Answer:
No.

9. Bias handling introduced during processing

Biases can, at least in theory, be introduced during processing. For example by nonlinear measurement equations in combination with large uncertainties on the input quantities. Is this something you try to correct for, or report, or deal with in some other way? Or do you think this will be negligible?

Answer:
Biases are introduced by calibration and forward model uncertainties. Bias correction on tb is provided for some sites (offset_tb). The propagation of this bias onto retrieved atmospheric TLWC may also be provided (clwvi_offset).

10. Other remarks on data product uncertainty

Please put here any other information about the data product uncertainty that you think is important.

Since MWRnet is an unfunded, bottom-up network, different levels of characterization are currently available among members. A common processing would significantly reduce this heterogeneity; activities towards this goal are ongoing but may not be totally implemented within the available dataset.

Annex I

GAIA-CLIM questionnaire about uncertainty in data products

FTIR – Ozone, methane and water vapour

Table of Contents

1. Identification of respondent and of data product

What are your contact details?

Answer:

Bavo Langerock
Belgian Institute for Space Aeronomy (BIRA-IASB)
Avenue circulaire 3
B-1180 Brussels
Belgium
Phone: +32/ 23736768
E-mail: bavo.langerock@aeronomie.be

For which data product are you filling in this questionnaire?

Answer:

FTIR NDACC O3 and CH4
FTIR MUSICA H2O

Please provide one or more accessible sources of information that a non-expert user can refer to, to gain an understanding of the measurement technique.

Answer:

de Mazière, M., etal., D4.2 NORS Data user guide, 2013, available as NORS deliverable at *http://nors.aeronomie.be/*, 2013

2. Recommended literature

*Which literature work would you recommend to understand better the measurement technique and the **general uncertainty framework** within which uncertainties of the data product are constructed. Note that for metrology, the vocabulary list of the VIM (*International Vocabulary of Metrology*), and the uncertainty framework of the GUM (Guide to expression of uncertainty) are important standards. Please provide a complete reference or doi where possible.*

Answer:

Rodgers, Inverse Methods for Atmospheric Sounding: Theory and Practice
Volume 2 van Series on atmospheric, oceanic and planetary physics, ISSN 1793-1452

*More specifically, which literature works (article, ATBD, other…) would you recommend to understand better how uncertainties of **this particular data product** are conceived? Please provide a complete reference or doi where possible.*

Answer:

Schneider, M and Hase, F, Technical Note: Recipe for monitoring of total ozone with a precision of around 1 DU applying mid-infrared solar absorption spectra, Atmospheric Chemistry and Physics, 2008(8)

See also the NDACC/FTIR Working group web page https://www2.acom.ucar.edu/irwg

Please specify also if the literature source is still up-to-date with the current data product. If not, where can a user find the information on the latest version of the data product and its uncertainties?

Answer: References mentioned above are still up-to-date.

3. Main measured quantity (measurand)

3.1 Specification of measurand

Specify the main measured quantities (i.e., the measurands) and the associated unit of the data product, along with their field name in the data product

Example measurands with unit: Temperature [K], O3 profile [ppmv], water vapour [ppmv]

Quantity [unit]	Field name
Volume mixing ratio [ppmv, ppbv]	[GAS].MIXING.RATIO.VOLUME_ABSORPTION.SOLAR
Total Column [molec/m^2]	[GAS].COLUMN_ABSORPTION.SOLAR
Volume mixing ratio [ppmv, ppbv]	H2O.ISO.MIXING.RATIO.VOLUME_ABSORPTION.SOLAR
Total Column [molec/m^2]	H2O.ISO.COLUMN_ABSORPTION.SOLAR

Where gas is any of the NDACC FTIR targets: O3 and CH4 (see https://www2.acom.ucar.edu/irwg for an up-to-date more extended list). H2O isotope data (see the H2O.ISO fields) is found in the MUSICA files.

3.2 Measurement equation

What is the relation between the main measured quantity of the data product and input quantities? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to literature publications).

Answer: The retrieval process or inversion (L1 L2) consists of extracting from the spectra the information about the absorbers' concentrations and vertical distributions in the atmosphere, based on the basic radiative transfer equations (Schwarzwild's equation). In the solar absorption case, Scharzwild's equation simplifies because the only radiation source to be considered is the sun, and in the infrared, one can omit scattering and therefore, the extinction coefficient reduces to the absorption coefficient.

The ‘inversion’ of this simplified Schwarzwild’s equation enables the determination of the absorbers’ concentrations, assuming perfect knowledge of the light path trajectory and of the absorption coefficients and their dependence on P and T.
In practice, the solution of the equation is not unequivocal (ill-posed problem) and some a priori knowledge must be used to find the most probable solution. The methods most often used at present are the Optimal Estimation Method and Tikhonov regularization [Rodgers, 2000]. The mathematics are shortly summarized in [ISSI, 2012].
The inversion then yields the retrieved vertical distribution x_r along the vertical (z) of the target absorber(s) in the atmosphere (Rodgers 2000):
$x_r = A(x_t - x_a) + x_a$, with x_t, the true profile, x_a the apriori information, A the AVK and x_r the retrieved profile.
A similar equation holds for column retrievals.

4. Traceability and comparability

4.1 SI or community traceability

Is the measurement quantity traceable, via an unbroken chain of processing steps, to SI units or community accepted standards?

Answer: Yes. See the traceability diagrams created within the GAIA-CLIM project. The measured quantity is an interferogram which is then Fourier transformed to an absorption spectrum in arbitrary units. From the shape of the absorption lines in selected micro-windows we can deduce information on targeted gas concentrations using optimal estimation.

If yes, please provide references to available literature describing the traceability aspects of the measurement.
De Mazière, M., et al., D4.2 NORS Data user guide, pp16-28, 2013, available as NORS deliverable at http://nors.aeronomie.be/

If no, please describe what aspects of the measurement are not fully traceable and how this aspect is addressed in deriving the data product and its uncertainty.

4.2 Comparability

If measurements are taken at multiple sites, are efforts made to ensure sufficiently similar measurement technique approaches to ensure comparability? Please provide links to any supporting materials available such as instrument manuals / network protocols.

Answer:
Some comparability can be achieved by cell measurements (Hase, 2012) or by atmospheric CO_2 measurements (Barthlott et al., 2015).

Hase, F.: Improved instrumental line shape monitoring for the ground-based, high-resolution FTIR spectrometers of the Network for the Detection of Atmospheric Composition Change, Atmos. Meas. Tech., 5, 603-610, doi:10.5194/amt-5-603-2012 , 2012.

Barthlott, S., M. Schneider, F. Hase, A. Wiegele, E. Christner, Y. González, T. Blumenstock, S. Dohe, O. E. García, E. Sepúlveda, K. Strong, J. Mendonca, D. Weaver, M. Palm, N. M. Deutscher, T. Warneke, J. Notholt, B. Lejeune, E. Mahieu, N. Jones, D. W. T. Griffith, V. A. Velazco, D. Smale, J. Robinson, R. Kivi, P. Heikkinen, and U. Raffalski: Using XCO2 retrievals for assessing the long-term consistency of NDACC/FTIR data sets, Atmos. Meas. Tech., 8, 1555-1573, doi:10.5194/amt-8-1555-2015, 2015

5. Representation of the uncertainty in the data product

5.1 Uncertainty field name(s)

Which field name(s) are used in the data product to hold the uncertainty value(s) associated with the main measured quantities? Note that more than one uncertainty field name can be associated with a single quantity (e.g., one field name for the "uncertainty due to random effects" and one for the "uncertainty due to systematic effects").

Field name of uncertainty	Associated quantity
[GAS].MIXING.RATIO.VOLUME_ABSORPTION.SOLAR_UNCERTAINTY.RANDOM.COVARIANCE	Random uncertainty matrix
[GAS].MIXING.RATIO.VOLUME_ABSORPTION.SOLAR_UNCERTAINTY.SYSTEMATIC.COVARIANCE	Systematic uncertainty matrix

5.2 Uncertainty form

In what form is the uncertainty per measurement represented in the data product? For example, is it:

- *A standard uncertainty (i.e., uncertainty expressed as standard deviation)*
- *A 95% coverage interval*
- *A variance-covariance matrix (if so, explain between which quantities the covariance is taken into account)*
- *A probability density function*
- *Other [please specify]*

Answer: The uncertainties are given as standard deviation and are reported as covariance matrices, containing correlations in the height axis. See also the uncertainty analysis as described in Rodgers 2000.

6. Uncertainty calculation

6.1 Formula/procedure

What is the formula/procedure by which the uncertainty is calculated? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to one or more equations in the literature).

Answer:
The details are provided in Rodgers 2000.

Is the uncertainty obtained by:

- *Uncertainty propagation, taking into account the uncertainties of the input quantities,*
- *Probability density function propagation,*
- *Sensitivity analysis: i.e., varying parameters and check the impact on the output quantity,*
- *Or still some other procedure?*

Answer:
Uncertainty propagation, taking into account the uncertainties of the input quantities.

6.2 Level of approximation

In what way is the uncertainty calculation procedure an approximation?

- *Is it based on (as is common practice) a first-order Taylor approximation (see GUM, Eq. (13))*

$$u_c^2(y)=\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i,x_j)=\sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i}\right)^2u^2(x_i)+2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i,x_j)$$

  which will not be exact if f is nonlinear.
- *Are correlations between input quantities neglected?*
- *Other approximations?*

Answer:
Taylor expansion.

If an approximation is involved, do you think the approximation can be a problem, or do you consider it justified?

Answer: Yes, because the system is assumed moderately non-linear around the retrieved state (cf Rodgers).

7. Uncertainty contributions

7.1 Prior

Is there a prior contribution? If so, is this prior based on measured data, a model, a rough guess, or something else?

Answer: Yes, we use prior information.
For MUSICA the prior information (mean state and covariance) are obtained from measurements (meteorological radiosondes) and models (especially the altitude dependent depletion of heavy water vapour isotopoplogues). It is the same for all sites and all time periods.

7.2 Smoothing error

Is an error source "smoothing error" included in the uncertainty calculation? If so, what do you define as "smoothing error"? Should the averaging kernel of the data product be applied in some way, before the uncertainty can be properly interpreted?

Answer: The smoothing is not part of the reported uncertainty budget.
The so-called smoothing error can be calculated by the user by means of the averaging kernel (cf Rodgers)

7.3 Noise

Is there a noise contribution? If so, what do you define as "noise"? (E.g., for MOPITT, one considers an instrumental noise, but also a "geophysical noise" (Deeter, 2013).)

Answer: Yes, noise is the random uncertainty on the measured spectrum .

7.4 Random and systematic contributions

Do you consider explicitly separately "random", "structured random" and "systematic" contributions? If so, how do you define each of these in your calculation?

Answer:
We distinguish random from systematic. Random represents the uncertainty component that decreases when averaging independent measurements (using the 1/√n rule). The systematic uncertainty does not decrease and the systematic uncertainty of an average is the average of the systematic uncertainties.

7.5 Input quantities / other parameters

If the main measured quantities of the data product depend on input quantities, how do the final uncertainties depend on uncertainties of these input quantities? Please provide a list with input quantities of which the uncertainties:

1. *Are taken into account.*

2. *Could be important, but are not taken into account. For example, because their consideration would be technically difficult, or it is not clear how to estimate the associated uncertainty.*
3. *Are not taken into account, as they can be demonstrated to be negligible.*

If this list is already available somewhere in a literature source, you can simply refer to it.

The dependency of final uncertainties on uncertainties of input quantities is taken into account. A list of assumed input uncertainties can be found, for instance, in Schneider and Hase (2008).

Schneider, M and Hase, F, Technical Note: Recipe for monitoring of total ozone with a precision of around 1 DU applying mid-infrared solar absorption spectra, Atmospheric Chemistry and Physics, 2008(8)

7.6 Uncertainty due to model error

Do you consider explicitly an uncertainty contribution due to the fact that the model is not perfect? Such uncertainty can be revealed e.g., by comparing results of several retrieval models.

Answer: No, but comparisons between different retrieval codes have been performed in the past (Hase et al., 2004).

Hase, F., J.W. Hannigan, M.T. Coffey, A. Goldman, M. Höpfner, N.B. Jones, C.P. Rinsland, S.W. Wood: Intercomparison of retrieval codes used for the analysis of high-resolution, ground-based FTIR measurements, Journal of Quantitative Spectroscopy & Radiative Transfer 87, 25–52, 2004.

8. Correlations/covariances

8.1 Presence in data product

Do you provide correlations or covariances within your data product, directly relevant to the main measured quantity? If so, between which quantities?

Answer: We provide altitude profiles and averaging kernels. The correlations between different altitudes can be deduced from the averaging kernels.

Please state in the table below which of the quantities are reported and/or included in the total error. Please use either yes, no or N/A for the first 2 columns and a short explanation in the 3rd. column. Add other quantities as relevant.

Quantity	Explicitly reported	Included in total error	Where reported / name given / comments

measurement noise covariance matrix		yes	
a priori covariance matrix			Not reported
Averaging kernel	yes		
Jacobian or K-matrix			Not reported

8.2 Auto-correlation

Suppose a user has to average several measured values of your data product. E.g., they want the mean column, 100 km around the observation site, within one month. Can you give a recommendation how they can obtain the uncertainty of this mean column, starting from the uncertainties provided for the individual columns?

Answer: see above. Random contributions should be averaged according to the $1/\sqrt{n}$ rule. Systematic uncertainties should be averaged arithmetically.

8.3 Correlation between main measured quantity and other quantities

Do you provide any correlation info between the main measured quantity (e.g., an ozone profile) and other quantities (e.g., a temperature profile)?

Answer: No.

9. Bias handling introduced during processing

Biases can, at least in theory, be introduced during processing. For example by nonlinear measurement equations in combination with large uncertainties on the input quantities. Is this something you try to correct for, or report, or deal with in some other way? Or do you think this will be negligible?

Answer: No. We think that this is likely negligible, see for instance Fig. 12 in Schneider et al., 2015).

Schneider, M., T. Blumenstock, F. Hase, M. Höpfner, E. Cuevas, A. Redondas, J.M. Sancho: Ozone profiles and total column amounts derived at Izaña Tenerife Island, from FTIR solar absorption spectra, and its validation by an intercomparison to ECC-sonde and Brewer spectrometer measurements, Journal of Quantitative Spectroscopy & Radiative Transfer 91, 245–274, 2005.

10. Other remarks on data product uncertainty

Please put here any other information about the data product uncertainty that you think is important.

Answer: In addition to theoretical uncertainty estimations, there is a variety of papers showing empirical uncertainty assessments by comparing the products to reference data. Below an incomplete list of examples:

Schneider, M., A. Redondas, F. Hase, C. Guirado, T. Blumenstock, and E. Cuevas: Comparison of ground-based Brewer and FTIR total column O3 monitoring techniques, ACP, Vol.8, 5535-5550, SRef-ID: 1680-7324/acp/2008-8-5535, 2008

Schneider, M., P. M. Romero, F. Hase, T. Blumenstock, E. Cuevas, and R. Ramos: Continuous quality assessment of atmospheric water vapour measurement techniques: FTIR, Cimel, MFRSR, GPS, and Vaisala RS92, Atmos. Meas. Tech., 3, 323-338, 2010.

García, O. E., M. Schneider, A. Redondas, Y. González, F. Hase, T. Blumenstock, and E. Sepúlveda: Investigating the long-term evolution of subtropical ozone profiles applying ground-based FTIR spectrometry, Atmos. Meas. Tech., 5, 2917-2931, doi:10.5194/amt-5-2917-2012, 2012

Sepúlveda, E., M. Schneider, F. Hase, S. Barthlott, D. Dubravica, O. E. García, A. Gomez-Pelaez, Y. González, J. C. Guerra, M. Gisi, R. Kohlhepp, S. Dohe, T. Blumenstock, K. Strong, D. Weaver, M. Palm, A. Sadeghi, N. M. Deutscher, T. Warneke, J. Notholt, N. Jones, D. W. T. Griffith, D. Smale, G. W. Brailsford, J. Robinson, F. Meinhardt, M. Steinbacher, T. Aalto, and D. Worthy: Tropospheric CH4 signals as observed by NDACC FTIR at globally distributed sites and comparison to GAW surface in-situ measurements, Atmos. Meas. Tech., 7, 2337-2360, doi:10.5194/amt-7-2337-2014, 2014.

Annex J

GAIA-CLIM questionnaire about uncertainty in data products

FTIR – Carbon dioxide and methane

Table of Contents

1. Identification of respondent and of data product

What are your contact details?

Answer:

Matthias Buschmann
Institute of Environmental Physics
University of Bremen - FB1
Postfach 330440
D-28334 Bremen
Germany

Phone: +49-421-218-62189
Email: m_buschmann@iup.physik.uni-bremen.de

For which data product are you filling in this questionnaire?

Answer:

FTIR TCCON CO2 and CH4

Please provide one or more accessible sources of information that a non-expert user can refer to, to gain an understanding of the measurement technique.

Answer:

Debra Wunch, Geoffrey C. Toon, Jean-François L. Blavier, Rebecca A. Washenfelder, Justus Notholt, Brian J. Connor, David W. T. Griffith, Vanessa Sherlock, Paul O. Wennberg, Phil. Trans. R. Soc. A 2011 369 2087-2112; DOI: 10.1098/rsta.2010.0240.

2. Recommended literature

*Which literature work would you recommend to understand better the measurement technique and the **general uncertainty framework** within which uncertainties of the data product are constructed. Note that for metrology, the vocabulary list of the VIM (*International Vocabulary of Metrology*), and the uncertainty framework of the GUM (Guide to expression of uncertainty) are important standards. Please provide a complete reference or doi where possible.*

Answer:

Wunch, D., G. C. Toon, V. Sherlock, N. M. Deutscher, X. Liu, D. G. Feist, and P. O. Wennberg. The Total Carbon Column Observing Network's GGG2014 Data Version. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, U.S.A. doi: 10.14291/tccon.ggg2014.documentation.R0/1221662, 2015.

More specifically, which literature works (article, ATBD, other…) would you recommend to understand better how uncertainties of ***this particular data product*** *are conceived? Please provide a complete reference or doi where possible.*

Answer: see citation above: Wunch et al. 2015

Please specify also if the literature source is still up-to-date with the current data product. If not, where can a user find the information on the latest version of the data product and its uncertainties?

Answer:
documentation refers to the current data product, also published via
http://tccon.ornl.gov/

3. Main measured quantity (measurand)

3.1 Specification of measurand

Specify the main measured quantities (i.e., the measurands) and the associated unit of the data product, along with their field name in the data product

Example measurands with unit: Temperature [K], O3 profile [ppmv], water vapour [ppmv]

Quantity [unit]	Field name
CO2 column averaged dry-air mole fraction [ppmv]	xco2
CH4 column averaged dry-air mole fraction [ppbv]	xch4

3.2 Measurement equation

What is the relation between the main measured quantity of the data product and input quantities? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to literature publications).

Answer:
The FTIR records an interferogram of direct solar light, which contains all spectral information. This interferogram is Fourier-tranformed into a spectrum. The actual retrieval process uses a priori information on trace gases to calculate a spectrum. The calculated spectrum is compared to the measured spectrum via a least-square fitting algorithm and the a priori information scaled in an iterative process which yields the target species trace gas concentration as a vertical column. The vertical column is then divided by the co-retrieved vertical column of oxygen and multiplied by the well-known atmospheric concentration of oxygen to yield the column averaged dry-air mole fraction (e.g. xCO2, xCH4).

Debra Wunch, Geoffrey C. Toon, Jean-François L. Blavier, Rebecca A. Washenfelder, Justus Notholt, Brian J. Connor, David W. T. Griffith, Vanessa Sherlock, Paul O. Wennberg
Phil. Trans. R. Soc. A 2011 369 2087-2112; DOI: 10.1098/rsta.2010.0240.

4. Traceability and comparability

4.1 SI or community traceability

Is the measurement quantity traceable, via an unbroken chain of processing steps, to SI units or community accepted standards?

Answer: Yes, see the GAIA-CLIM traceability diagram for FTIR TCCON measurements.

If yes, please provide references to available literature describing the traceability aspects of the measurement.

The latest collection of all WMO-standard traceable aircraft comparisons can be found in

Wunch, D., G. C. Toon, V. Sherlock, N. M. Deutscher, X. Liu, D. G. Feist, and P. O. Wennberg. The Total Carbon Column Observing Network's GGG2014 Data Version. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, U.S.A. doi: 10.14291/tccon.ggg2014.documentation.R0/1221662, 2015.

If no, please describe what aspects of the measurement are not fully traceable and how this aspect is addressed in deriving the data product and its uncertainty.

4.2 Comparability

If measurements are taken at multiple sites, are efforts made to ensure sufficiently similar measurement technique approaches to ensure comparability? Please provide links to any supporting materials available such as instrument manuals / network protocols.

Answer:
Yes, comparability is proven by co-located aircraft profiles, side by side measurements and furthermore instrument stability is routinely monitored via gas cell measurements.

5. Representation of the uncertainty in the data product

5.1 Uncertainty field name(s)

Which field name(s) are used in the data product to hold the uncertainty value(s) associated with the main measured quantities? Note that more than one uncertainty field name can be associated with a single quantity (e.g., one field name for the “uncertainty due to random effects” and one for the “uncertainty due to systematic effects”).

Field name of uncertainty	Associated quantity
xco2_error	Random error
xch4_error	Random error

5.2 Uncertainty form

In what form is the uncertainty per measurement represented in the data product? For example, is it:

- *A standard uncertainty (i.e., uncertainty expressed as standard deviation)*
- *A 95% coverage interval*
- *A variance-covariance matrix (if so, explain between which quantities the covariance is taken into account)*
- *A probability density function*
- *Other [please specify]*

Answer: Random error from the retrieval processing code, associated with spectral noise
Note that the systematic error is minimized by in-situ calibration within the data post-processing.

6. Uncertainty calculation

6.1 Formula/procedure

What is the formula/procedure by which the uncertainty is calculated? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to one or more equations in the literature).

Answer:

Two types of errors are considered. Random error, originating from the residuum of the calculated and measured spectrum after the least-square fitting is applied. This error is reported as part of the official TCCON data product. The systematic error sources are dealt with, by implementation of an in-situ-correction scheme.

As it is not possible to trace the errors of input parameters through the retrieval algorithm of the dry-air mole fractions, sensitivity studies have been performed. These have been done by independently changing various potential sources of error using conservative estimates and analysing the change in retrieved xCO2 and xCH4.

Is the uncertainty obtained by:

- *Uncertainty propagation, taking into account the uncertainties of the input quantities,*
- *Probability density function propagation,*
- *Sensitivity analysis: i.e., varying parameters and check the impact on the output quantity,*
- *Or still some other procedure?*

Answer:
A sensitivity analysis for various input parameters has been performed and is shown in:

Wunch, D., G. C. Toon, V. Sherlock, N. M. Deutscher, X. Liu, D. G. Feist, and P. O. Wennberg. The Total Carbon Column Observing Network's GGG2014 Data Version. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, U.S.A. doi: 10.14291/tccon.ggg2014.documentation.R0/1221662, 2015.

6.2 Level of approximation

In what way is the uncertainty calculation procedure an approximation?

- *Is it based on (as is common practice) a first-order Taylor approximation (see GUM, Eq. (13))*

$$u_c^2(y) = \sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i, x_j) = \sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i, x_j)$$

  which will not be exact if f is nonlinear.
- *Are correlations between input quantities neglected?*
- *Other approximations?*

Answer:
The outcome of the above mentioned sensitivity study depends on assumptions of the error of input parameters. Care has been taken to choose adequate estimates.

If an approximation is involved, do you think the approximation can be a problem, or do you consider it justified?

Answer:
The uncertainties caused by approximations do not cause a problem, their impact is estimated conservatively.

7. Uncertainty contributions

7.1 Prior

Is there a prior contribution? If so, is this prior based on measured data, a model, a rough guess, or something else?

Answer:
Yes, an a priori gas profile is scaled by the retrieval algorithm. It is based on measured data for CH4. For CO2 the prior is calculated by an empirical model of the xCO2, including secular trend and seasonal cycle.

7.2 Smoothing error

Is an error source "smoothing error" included in the uncertainty calculation? If so, what do you define as "smoothing error"? Should the averaging kernel of the data product be applied in some way, before the uncertainty can be properly interpreted?

Answer:
Priors and averaging kernels are shipped with the data product. Averaging kernel smoothing has to be done, before comparing to other data products.

7.3 Noise

Is there a noise contribution? If so, what do you define as "noise"? (E.g., for MOPITT, one considers an instrumental noise, but also a "geophysical noise" (Deeter, 2013).)

Answer:
Photon noise and electronic noise are treated together as spectral noise and are reflected in the measurand error.

7.4 Random and systematic contributions

Do you consider explicitly separately "random", "structured random" and "systematic" contributions? If so, how do you define each of these in your calculation?

Answer:
Only the random error is reported in the data product. Systematic bias is treated separately in post processing.

7.5 Input quantities / other parameters

If the main measured quantities of the data product depend on input quantities, how do the final uncertainties depend on uncertainties of these input quantities? Please provide a list with input quantities of which the uncertainties:

1. *Are taken into account.*
2. *Could be important, but are not taken into account. For example, because their consideration would be technically difficult, or it is not clear how to estimate the associated uncertainty.*
3. *Are not taken into account, as they can be demonstrated to be negligible.*

If this list is already available somewhere in a literature source, you can simply refer to it.

See sensitivity study in

Wunch, D., G. C. Toon, V. Sherlock, N. M. Deutscher, X. Liu, D. G. Feist, and P. O. Wennberg. The Total Carbon Column Observing Network's GGG2014 Data Version. Carbon Dioxide Information

Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, U.S.A. doi: 10.14291/tccon.ggg2014.documentation.R0/1221662, 2015.

7.6 Uncertainty due to model error

Do you consider explicitly an uncertainty contribution due to the fact that the model is not perfect? Such uncertainty can be revealed e.g., by comparing results of several retrieval models.

Answer:
The model might not be perfect (wrong spectral data or simplified radiative transfer calculations) but due to the validation by independent methods such potential errors are considered.

8. Correlations/covariances

8.1 Presence in data product

Do you provide correlations or covariances within your data product, directly relevant to the main measured quantity? If so, between which quantities?

Answer: No, averaging kernels are shipped with the product, but not considered in error estimation, because AK smoothing is expected from the user.

8.2 Auto-correlation

Suppose a user has to average several measured values of your data product. E.g., they want the mean column, 100 km around the observation site, within one month. Can you give a recommendation how they can obtain the uncertainty of this mean column, starting from the uncertainties provided for the individual columns?

Answer:
Within TCCON the distance from one site to the next is more than 100 km, this will not occur. If the users think of averaging results from different sites, the different concentrations at two sites are much higher than the uncertainties of the individual sites.

8.3 Correlation between main measured quantity and other quantities

Do you provide any correlation info between the main measured quantity (e.g., an ozone profile) and other quantities (e.g., a temperature profile)?

Answer: No.

9. Bias handling introduced during processing

Biases can, at least in theory, be introduced during processing. For example by nonlinear measurement equations in combination with large uncertainties on the input quantities. Is this *something you try to correct for, or report, or deal with in some other way? Or do you think this will be negligible?*

Answer:
We believe that a potential bias is minimized due to the aircraft validation.

10. Other remarks on data product uncertainty

Please put here any other information about the data product uncertainty that you think is important.

Annex K

GAIA-CLIM questionnaire about uncertainty in data products

UV-VIS – Total ozone column

Table of Contents

1. Identification of respondent and of data product

What are your contact details?

Answer:

Francois Hendrick
Belgian Institute for Space Aeronomy (BIRA-IASB)
Avenue circulaire, 3, B-1180 Brussels, Belgium
Phone: +32/(0)2-373 67 66
E-mail: francois.hendrick@aeronomie.be

For which data product are you filling in this questionnaire?

Answer:

Total O_3 column densities from twilight ground-based DOAS UV-vis measurements

Please provide one or more accessible sources of information that a non-expert user can refer to, to gain an understanding of the measurement technique.

De Mazière, M., et al., D4.2 NORS Data user guide, pp16-28, 2013, available as NORS deliverable at http://nors.aeronomie.be/.

2. Recommended literature

*Which literature work would you recommend to understand better the measurement technique and the **general uncertainty framework** within which uncertainties of the data product are constructed. Note that for metrology, the vocabulary list of the VIM (*International Vocabulary of Metrology*) and the uncertainty framework of the GUM (Guide to expression of uncertainty) are important standards. Please provide a complete reference or doi where possible.*

Answer:

Platt, U. and Stutz, J., Differential Optical Absorption Spectroscopy (DOAS), Principles and Applications, ISBN 978-3-540-21193-8, Springer, Berlin-Heidelberg, 2008.

*More specifically, which literature works (article, ATBD, other…) would you recommend to understand better how uncertainties of **this particular data product** are conceived? Please provide a complete reference or doi where possible.*

Hendrick, F., J.-P. Pommereau, F. Goutail, R. D. Evans, D. Ionov, A. Pazmino, E. Kyrö, G. Held, P. Eriksen, V. Dorokhov, M. Gil, and M. Van Roozendael, NDACC/SAOZ UV-visible total ozone

measurements: Improved retrieval and comparison with correlative ground-based and satellite observations, Atmos. Chem. Phys., 11, 5975-5995, 2011.

See also the NDACC/UV-vis Working Group web page available at http://ndacc-uvvis-wg.aeronomie.be/tools.php

Please specify also if the literature source is still up-to-date with the current data product. If not, where can a user find the information on the latest version of the data product and its uncertainties?

Answer:
References mentioned above are still up-to-date.

3. Main measured quantity (measurand)

3.1 Specification of measurand

Specify the main measured quantities (i.e., the measurands) and the associated unit of the data product, along with their field name in the data product

Example measurands with unit: Temperature [K], O3 profile [ppmv], water vapour [ppmv]

Quantity [unit]	Field name
O_3 total vertical column [molec./cm2]	**O3.COLUMN.STRATOSPHERIC_SCATTER.SOLAR.ZENITH**

3.2 Measurement equation

What is the relation between the main measured quantity of the data product and input quantities? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to literature publications).

Answer:
The total O_3 column density retrieval from twilight ground-based DOAS UV-vis measurements is described in details in both references above. In brief, O_3 is retrieved in the visible Chappuis bands in a wavelength range of about 100 nm wide centered around 500 nm, taking into account the spectral signature of O_3, NO_2, H_2O, O_4, and the filling-in of the solar Fraunhofer bands by the Ring effect (Grainger and Ring, 1962).

The O_3 differential slant column density (DSCD), which is the amount of O_3 present in the optical path that the light follows to the instrument minus that from a reference measurement, is the direct product of the DOAS spectral analysis. It is converted into a vertical column amount using the following equation:

$$VCD(\theta) = \frac{DSCD(\theta) + RCD}{AMF(\theta)} \quad \textbf{(1)}$$

where *VCD(θ)* is the vertical column density at SZA θ, *DSCD(θ)* the differential slant column density at SZA θ, *RCD* the residual ozone amount in the reference measurement (a fixed spectrum recorded at high sun around local noon), and *AMF(θ)* the airmass factor at SZA θ.

RCD is derived using the so-called Langley plot method, which consists in rearranging Eq. 1 and plotting *DSCD(θ)* as a function of *AMF(θ)*, the intercept at AMF = 0 giving *RCD* (Roscoe et al., 1994; Vaughan et al., 1997). Sunrise and sunset O_3 column data provided to the NDACC database are derived by averaging vertical columns estimated with Eq. 1 over a limited SZA range around 90°SZA (generally 86-91° SZA). The AMF, also called geometrical enhancement, is defined as the ratio between the slant and vertical column densities (Solomon et al., 1987). O_3 AMF are extracted from the NDACC look-up tables generated using the UVSPEC/DISORT radiative transfer model (Mayer and Kylling, 2005) and the following input parameters:

Parameter	Value
O_3 profile	TOMS version 8 O_3 profile climatology (McPeters et al., 2007): - Latitude: 85°S to 85°N step 10° - Month: 1 (Jan) to 12 (Dec) step 1 - Ozone column: 125 to 575 DU step 50 DU
Pressure, temperature profiles	TOMS version 8 O_3 profile climatology (McPeters et al., 2007):
Altitude grid	0-120km/step 1km
Wavelength	440 to 580 nm step 35 nm
Surface albedo	0 and 1
Station altitude	0 and 4 km
SZA	10, 30, 50, 70, 80, 82.5, 85, 86, 87, 88, 89, 90, 91, and 92°

Table 1: Parameter values for which the LUTs were calculated.

Grainger, J. and Ring, J.: Anomalous Fraunhofer line profiles, Nature, 193, 762, 1962.

Mayer, B. and Kylling, A.: Technical note: The LibRadtran software package for radiative transfer calculations – Description and examples of use, Atmos. Chem. Phys., 5, 1855–1877, 2005.

McPeters, R. D., Labow, G. J., and Logan, J. A.: Ozone climatological profiles for satellite retrieval algorithms, J. Geophys. Res., 112, D05308, doi:10.1029/2005JD006823, 2007.

Roscoe, H. K., Squires, J. A. C., Oldham, D. J., Sarkissian, A., Pommereau, J.-P., and Goutail, F.: Improvements to the accuracy of zenith-sky measurements of total ozone by visible spectrometers, J. Quant. Spectrosc. Radiat. Transfer, 52(5), 639-648, 1994.

Vaughan, G., Roscoe, H. K., Bartlett, L. M., O'Connor, F., Sarkissian, A., Van Roozendael, M., Lambert, J.-C., Simon, P. C., Karlsen, K., Kaestad Hoiskar, B. A., Fish, D. J., Jones, R. L., Freshwater, R., Pommereau, J.-P., Goutail, F., Andersen, S. B., Drew, D. G., Hughes, P. A., Moore, D., Mellqvist, J., Hegels, E., Klupfel, T., Erle, F., Pfeilsticker, K., and Platt, U.: An intercomparison of ground-based UV-visible sensors of ozone and NO_2, J. Geophys. Res., 102, 1411-1422, 1997.

4. Traceability and comparability

4.1 SI or community traceability

Is the measurement quantity traceable, via an unbroken chain of processing steps, to SI units or community accepted standards?

Answer:
Yes. The corresponding traceability chain has been developed in the framework of the GAIA-CLIM project, as part of WP2.

If yes, please provide references to available literature describing the traceability aspects of the measurement.

Hendrick, F., J.-P. Pommereau, F. Goutail, R. D. Evans, D. Ionov, A. Pazmino, E. Kyrö, G. Held, P. Eriksen, V. Dorokhov, M. Gil, and M. Van Roozendael, NDACC/SAOZ UV-visible total ozone measurements: Improved retrieval and comparison with correlative ground-based and satellite observations, Atmos. Chem. Phys., 11, 5975-5995, 2011.

De Mazière, M., et al., D4.2 NORS Data user guide, pp16-28, 2013, available as NORS deliverable at http://nors.aeronomie.be/.

NDACC/UV-vis Working Group web page available at http://ndacc-uvvis-wg.aeronomie.be/tools.php

If no, please describe what aspects of the measurement are not fully traceable and how this aspect is addressed in deriving the data product and its uncertainty.

4.2 Comparability

If measurements are taken at multiple sites, are efforts made to ensure sufficiently similar measurement technique approaches to ensure comparability? Please provide links to any supporting materials available such as instrument manuals / network protocols.

Answer:
A harmonisation effort of total O_3 column retrieval has been carried within the framework of the NDACC UV-vis Working Group. Recommendations on retrieval procedure and settings can be found at http://ndacc-uvvis-wg.aeronomie.be/tools.php. It has been also decided to adopt the GEOMS HDF data file format which allows a high level of traceability for the different reported variables. The corresponding template can be found at http://avdc.gsfc.nasa.gov/index.php?site=1876901039.

5. Representation of the uncertainty in the data product

5.1 Uncertainty field name(s)

Which field name(s) are used in the data product to hold the uncertainty value(s) associated with the main measured quantities? Note that more than one uncertainty field name can be associated *with a single quantity (e.g., one field name for the "uncertainty due to random effects" and one for the "uncertainty due to systematic effects").*

Field name of uncertainty	Associated quantity
O3.COLUMN.STRATOSPHERIC_SCATTER.SOLAR.ZENITH_UNCERTAINTY.RANDOM.STANDARD	Random uncertainty on O_3 VCD
O3.COLUMN.STRATOSPHERIC_SCATTER.SOLAR.ZENITH_UNCERTAINTY.SYSTEMATIC.STANDARD	Systematic uncertainty on O_3 VCD

5.2 Uncertainty form

In what form is the uncertainty per measurement represented in the data product? For example, is it:

- *A standard uncertainty (i.e., uncertainty expressed as standard deviation)*
- *A 95% coverage interval*
- *A variance-covariance matrix (if so, explain between which quantities the covariance is taken into account)*
- *A probability density function*
- *Other [please specify]*

Answer:
Standard uncertainties

6. Uncertainty calculation

6.1 Formula/procedure

What is the formula/procedure by which the uncertainty is calculated? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to one or more equations in the literature).

Is the uncertainty obtained by:

- *Uncertainty propagation, taking into account the uncertainties of the input quantities,*
- *Probability density function propagation,*
- *Sensitivity analysis: i.e., varying parameters and check the impact on the output quantity,*
- *Or still some other procedure?*

Answer:
The uncertainty budget on twilight UV-vis O_3 VCDs is described Hendrick et al. (2011). We give here only a short summary, separating the random and systematic uncertainties for the three main retrieval steps (spectral fit, determination of the residual amount in the reference spectra (RCD) and AMF extraction/calculation):

-Random uncertainty on O_3 DSCDs (spectral fit):

DOAS random errors are mostly related to the measurement noise which for silicon array detectors is generally limited by the photon shot noise. Assuming uncorrelated errors for the individual detector pixels and if the DOAS fit residuals are dominated by instrumental noise, the random contribution to the DSCD error can be derived from the DOAS least-squares fit error propagation (see e.g. Stutz and Platt, 2008), and the random errors are represented by the slant column DOAS fit RMS.

-Systematic uncertainty on O_3 DSCDs (spectral fit):

The main sources of systematic uncertainties related to the DOAS spectral fit are the uncertainties on the cross-sections (trace gases + Ring effect), as well as the calibration uncertainties (mainly slit function and wavelength calibration). These uncertainties are estimated using sensitivity analysis (e.g. changing the cross-section sources and quantify the impact on the retrieved DSCDs), assuming uncorrelated effects between the tested parameters. The total systematic uncertainty on DSCDs is calculated by adding the different uncertainty sources in Gaussian quadrature.

-Random uncertainty on O_3 RCD (determination of the residual amount in the reference spectra):

RCD is determined using the Langley-plot approach, i.e. a linear regression analysis method. The random uncertainty on O_3 RCD corresponds to the 1-sigma standard deviation on the calculated intercept.

-Systematic uncertainty on O_3 RCD (determination of the residual amount in the reference spectra):

No systematic uncertainty is considered here.

-Random uncertainty on O_3 AMFs:

The random uncertainties on the O_3 and AMFs are estimated based on sensitivity tests on the main parameters affecting the AMF calculation and/or extraction, which are (see Hendrick et al., 2011): O_3 and aerosol extinction vertical profiles, surface albedo, clouds, and the choice of the radiative transfer model used to calculate the AMFs. The corresponding uncertainties are derived by varying these parameters and quantifying the impact of the changes on the extracted AMFs, assuming uncorrelated effects between the tested parameters. The total random uncertainty on AMFs is calculated by adding the different uncertainty sources in Gaussian quadrature.

-Systematic uncertainty on O_3 AMFs:

No systematic uncertainty is considered here.

The total random and systematic uncertainties reported in the UV-vis total O_3 column data files are estimated by adding in quadrature the corresponding uncertainty sources for DSCDs, RCDs, and AMFs.

6.2 Level of approximation

In what way is the uncertainty calculation procedure an approximation?

- *Is it based on (as is common practice) a first-order Taylor approximation (see GUM, Eq. (13))*

$$u_c^2(y)=\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i,x_j)=\sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i)+2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i,x_j)$$

  which will not be exact if f is nonlinear.
- *Are correlations between input quantities neglected?*
- *Other approximations?*

If an approximation is involved, do you think the approximation can be a problem, or do you consider it justified?

Answer:
The adopted approach which is a sensitivity analysis on main parameters affecting the spectral fit and AMF calculation/extraction assuming no correlation between the tested parameters can be considered as an approximation. This is the common approach followed so far by the NDACC UV-vis Working Group.

7. Uncertainty contributions

7.1 Prior

Is there a prior contribution? If so, is this prior based on measured data, a model, a rough guess, or something else?

Answer:
Yes. Trace gas cross-sections, O_3 AMF LUTs and associated surface albedo climatology (see Sections 3 and 5).

7.2 Smoothing error

Is an error source "smoothing error" included in the uncertainty calculation? If so, what do you define as "smoothing error"? Should the averaging kernel of the data product be applied in some way, before the uncertainty can be properly interpreted?

Answer:
There is no smoothing error included in the uncertainty calculation.

Column averaging kernels (AVK) are provided in the total O_3 column data files. They are extracted from column AVK LUTs calculated from the Eskes and Boersma (2003)'s approach, using the UVSPEC/DISORT radiative transfer model initialized with similar parameter values as for the AMF LUTs calculation (see Table 1 in Section 3).

Eskes, H. and Boersma, K. F., Averaging kernels for DOAS total-column satellite retrievals, Atmos. Chem. Phys., 1285–1291, 2003.

7.3 Noise

Is there a noise contribution? If so, what do you define as "noise"? (E.g., for MOPITT, one considers an instrumental noise, but also a "geophysical noise" (Deeter, 2013).)

Answer: Yes, see Section 6.1.

7.4 Random and systematic contributions

Do you consider explicitly separately "random", "structured random" and "systematic" contributions? If so, how do you define each of these in your calculation?

Answer: Yes, see Section 6.1. Random and systematic contributions are defined as in Section 10.2 of the present document.

7.5 Input quantities / other parameters

If the main measured quantities of the data product depend on input quantities, how do the final uncertainties depend on uncertainties of these input quantities? Please provide a list with input quantities of which the uncertainties:

1. *Are taken into account.*
2. *Could be important, but are not taken into account. For example, because their consideration would be technically difficult, or it is not clear how to estimate the associated uncertainty.*
3. *Are not taken into account, as they can be demonstrated to be negligible.*

If this list is already available somewhere in a literature source, you can simply refer to it.

Answer: See Section 6.1.

Input quantity/other parameter	associated uncertainty or "important but ignored" or "negligible"	Extra info (e.g., random, systematic)
Cross-section data sets	Important	Systematic
O_3 AMF LUTs and related surface albedo climatology	Important	Random

7.6 Uncertainty due to model error

Do you consider explicitly an uncertainty contribution due to the fact that the model is not perfect? Such uncertainty can be revealed e.g., by comparing results of several retrieval models.

Answer: Yes, the uncertainty of the AMF LUT calculation/extraction and trace gases cross-sections are taken into account in the uncertainties estimate (see Section 6.1).

8. Correlations/covariances

8.1 Presence in data product

Do you provide correlations or covariances within your data product, directly relevant to the main measured quantity? If so, between which quantities?

Answer: No.

Please state in the table below which of the quantities are reported and/or included in the total error. Please use either yes, no or N/A for the first 2 columns and a short explanation in the 3rd. column. Add other quantities as relevant.

Quantity	Explicitly reported	Included in total error	Where reported / name given / comments
measurement noise covariance matrix	No	No	
a priori covariance matrix	No	No	
Averaging kernel	Yes	No	
Jacobian or K-matrix	No	No	

8.2 Auto-correlation

Suppose a user has to average several measured values of your data product. E.g., they want the mean column, 100 km around the observation site, within one month. Can you give a recommendation how they can obtain the uncertainty of this mean column, starting from the uncertainties provided for the individual columns?

Answer: No.

8.3 Correlation between main measured quantity and other quantities

Do you provide any correlation info between the main measured quantity (e.g., an ozone profile) and other quantities (e.g., a temperature profile)?

Answer: No.

9. Bias handling introduced during processing

Biases can, at least in theory, be introduced during processing. For example by nonlinear measurement equations in combination with large uncertainties on the input quantities. Is this something you try to correct for, or report, or deal with in some other way? Or do you think this will be negligible?

Answer: Possible biases are not taken into account in the uncertainty budget evaluation.

10. Other remarks on data product uncertainty

Please put here any other information about the data product uncertainty that you think is important.

Annex L

GAIA-CLIM questionnaire about uncertainty in data products

Dobson – Total column ozone

Table of Contents

1. Identification of respondent and of data product

What are your contact details?

Answer:
Karin Kreher
BK Scientific GmbH
Astheimerweg 42
D-55130 Mainz
Germany
Email: karin.kreher@bkscientific.eu

Expert feed-back and advice was provided by the Dobson community, in particular by Irina Petropavlovskikh and Luca Egli.

For which data product are you filling in this questionnaire?

Answer: Total ozone column from direct sun Dobson measurements

Please provide one or more accessible sources of information that a non-expert user can refer to, to gain an understanding of the measurement technique.

Answer:
Vanicek, K.: Differences between ground Dobson, Brewer and satellite TOMS-8, GOME-WFDOAS total ozone observations at Hradec Kralove, Czech, Atmos. Chem. Phys., 6, 5163-5171, doi:10.5194/acp-6-5163-2006, 2006. http://www.atmos-chem-phys.net/6/5163/2006/acp-6-5163-2006.pdf

2. Recommended literature

*Which literature work would you recommend to understand better the measurement technique and the **general uncertainty framework** within which uncertainties of the data product are constructed. Note that for metrology, the vocabulary list of the VIM (*International Vocabulary of Metrology*) and the uncertainty framework of the GUM (Guide to expression of uncertainty) are important standards. Please provide a complete reference or doi where possible.*

Answer:
1) WMO report #183, OPERATIONS HANDBOOK – OZONE OBSERVATIONS WITH A DOBSON SPECTROPHOTOMETER. by W. D. Komhyr, 1980, Revised in 2008 by Robert D. Evans
http://www.wmo.int/pages/prog/arep/gaw/documents/GAW183-Dobson-WEB.pdf

2) Evaluation of Dobson and Brewer total ozone observations from Hradec Králové Czech Republic, 1961-2002. Report of the project CANDIDOZ, Working group WG-1, 5-th RTD Framework Programme, Project No.: EVK2-2001-00024
By Karel Vaníček, Martin Staněk, and Martin Dubrovský
http://www.o3soft.eu/dobsonweb/messages/vanicekd074reeval.pdf

*More specifically, which literature works (article, ATBD, other…) would you recommend to understand better how uncertainties of **this particular data product** are conceived? Please provide a complete reference or doi where possible.*

Answer:
The Ozone ad-hoc group webpage has a compilation of papers that describe the Dobson instrument, its calibration, data quality and comparisons with other ozone-monitoring instruments
http://www.o3soft.eu/dobsonweb/papers.html

Please specify also if the literature source is still up-to-date with the current data product. If not, where can a user find the information on the latest version of the data product and its uncertainties?

Answer:
Preliminary results of a software tool to roughly estimate the uncertainties of retrieving TOC from Dobson, Brewer and Array-Spectroradiometer measurements are presented in a power point presentation on the webpage of the Joint Research Project "Traceability for atmospheric total columne ozone".
"A simulation tool to model ozone retrieval uncertainties of Brewer and Dobson instruments" By Luca Egli Julian Gröbner, Ulf Köhler, Alberto Redondas, Virgilio Carreño and Henri Diemoz ("UVNews-Team"), Mario Blumthaler, Omar El Gawhary, Petri Kärhä, Ingo Kröger and Mark Weber ("ATMOZ Uncertainty Team")
https://projects.pmodwrc.ch/atmoz/images/ATMOZ_forum/12_Egli.pdf

Please note that these results are preliminary and they are based on model calculations. A comprehensive uncertainty budget, tested with measurements from 2 measurement campaigns, will be made available in October 2017.

3. Main measured quantity (measurand)

3.1 Specification of measurand

Specify the main measured quantities (i.e., the measurands) and the associated unit of the data product, along with their field name in the data product

Example measurands with unit: Temperature [K], O3 profile [ppmv], water vapour [ppmv]

Quantity [unit]	Field name
mili-atm-cm or DU	Dobson Unit

3.2 Measurement equation

What is the relation between the main measured quantity of the data product and input quantities? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to literature publications).

Answer:
Detailed information concerning derivation of the mathematical equations used in reducing total ozone measurement data obtained from observations on direct sun or moon are given in Dobson (1957a, 1957b).

Measurement of total column ozone in the atmosphere with the Dobson ozone spectrophotometer comes out from the equation of attenuation of the solar ultraviolet radiation by key atmospheric constituents at two sets of wavelengths in the Solar UV and visible spectra.

$N = L_0 - L = \log(I_0 / I'_0) - \log(I / I')$

I_0 and I_0' … intensities outside the atmosphere of solar radiation at the short and long wavelengths, respectively, of the wavelength pair;
I and I' … measured intensities at the ground of solar radiation at the short and long wavelengths, respectively;

$\log I = \log I_0 - \alpha\ \mu\ O_3 - \beta\ m\ P/P_o - \delta \sec ZA$

where:
I_0 ... spectral intensity outside the atmosphere (extra-terrestrial)
I ... spectral intensity of solar radiation at the ground
O_3 ... total amount of ozone in the atmosphere in Dobson Units (mili-atm-cm)
ZA ... zenith angle of the Sun
m ... relative path of the solar radiation through the atmosphere
P ... observed air pressure at the ground
P_o ... mean sea level pressure
α ... spectral absorption coefficient of ozone
β ... spectral Rayleigh molecular scattering coefficients of the air
δ ... spectral scattering coefficients of aerosol particles
μ ... relative path of the solar radiation through the ozone layer

Dobson, G. M. B., Observers' Handbook for the Ozone Spectrophotometer, in Annals of the International Geophysical Year, V, Part 1, 46-89, Pergamon Press, 1957a.
Dobson, G. M. B., Adjustment and Calibration of the Ozone Spectrophotometer, ibid. V, Part I, 90-113, Pergamon Press, 1957b.

4. Traceability and comparability

4.1 SI or community traceability

Is the measurement quantity traceable, via an unbroken chain of processing steps, to SI units or community accepted standards?

Answer:
Yes. The corresponding traceability chain has been developed in the framework of the WMO GAW Dobson network, with reference to the WMO Dobson standard instrument # 083.

If yes, please provide references to available literature describing the traceability aspects of the measurement.

The Ozone ad-hoc group webpage has a compilation of papers that describe Dobson instrument, its calibration, data quality and comparisons with other ozone-monitoring instruments
http://www.o3soft.eu/dobsonweb/papers.html

If no, please describe what aspects of the measurement are not fully traceable and how this aspect is addressed in deriving the data product and its uncertainty.

4.2 Comparability

If measurements are taken at multiple sites, are efforts made to ensure sufficiently similar measurement technique approaches to ensure comparability? Please provide links to any supporting materials available such as instrument manuals / network protocols.

Answer:
Yes. All operators follow the guidelines described in the WMO report #183, OPERATIONS HANDBOOK – OZONE OBSERVATIONS WITH A DOBSON SPECTROPHOTOMETER. by W. D. Komhyr, 1980, Revised in 2008 by Robert D. Evans
http://www.wmo.int/pages/prog/arep/gaw/documents/GAW183-Dobson-WEB.pdf

5. Representation of the uncertainty in the data product

5.1 Uncertainty field name(s)

Which field name(s) are used in the data product to hold the uncertainty value(s) associated with the main measured quantities? Note that more than one uncertainty field name can be associated with a single quantity (e.g., one field name for the "uncertainty due to random effects" and one for the "uncertainty due to systematic effects").

Please note that the results in the table below are preliminary and they are based on model calculations. A comprehensive uncertainty budget, tested with measurements from 2 measurement campaigns will be available in October 2017 and can be requested from the ATMOZ website: http://projects.pmodwrc.ch/atmoz/

Field name of uncertainty	Associated quantity
Systematic uncertainty 0.14-0.3 %	
Total uncertainty (all parameters below)	1.7%
Wavelength registration ±0.025 nm	0.1%
Noise of detector /Calibration /ND filter Dead-time /linearity/ Instr. Temperature ±0.1%	0.06%
Strat. Temp Bass-Paur: 213K-243 K	1.2%
Strat. Temp Bremen: 213K-243 K	0.6%
Cross-Section Bass-Paur:+/- 5%	1.2%
Extra-terrestrial:+/- 5%	0%
Ozone air mass variation	liner
AOD/SO2	Not determined yet

5.2 Uncertainty form

In what form is the uncertainty per measurement represented in the data product? For example, is it:

- *A standard uncertainty (i.e., uncertainty expressed as standard deviation)*
- *A 95% coverage interval*
- *A variance-covariance matrix (if so, explain between which quantities the covariance is taken into account)*
- *A probability density function*
- *Other [please specify]*

Answer: The uncertainty form in the table above are standard uncertainties.

6. Uncertainty calculation

6.1 Formula/procedure

What is the formula/procedure by which the uncertainty is calculated? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to one or more equations in the literature).

Answer:
Random variation of parameters in the ozone equation
$O_3 = (N - (\beta_1 - \beta_2)\, m\, P/P_o - (\delta_1 - \delta_2)\, \sec ZA) / (\alpha_1 - \alpha_2)\, \mu$

Is the uncertainty obtained by:

- *Uncertainty propagation, taking into account the uncertainties of the input quantities,*

- *Probability density function propagation,*
- *Sensitivity analysis: i.e., varying parameters and check the impact on the output quantity,*
- *Or still some other procedure?*

Answer:
Yes, the uncertainties are obtained by Monte-Carlo ensemble simulations. However - in the ATMOZ project also other approaches will be investigated.

6.2 Level of approximation

In what way is the uncertainty calculation procedure an approximation?

- *Is it based on (as is common practice) a first-order Taylor approximation (see GUM, Eq. (13))*

$$u_c^2(y) = \sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i, x_j) = \sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i, x_j)$$

  which will not be exact if f is nonlinear.
- *Are correlations between input quantities neglected?*
- *Other approximations?*

Answer: Yes.

If an approximation is involved, do you think the approximation can be a problem, or do you consider it justified?

Answer: N/A

7. Uncertainty contributions

7.1 Prior

Is there a prior contribution? If so, is this prior based on measured data, a model, a rough guess, or something else?

Answer:
All Dobson spectrophotometers use the values of α determined for the slit function of the World Primary Dobson Spectrophotometer D083 (WPSS) and effective ozone temperature TOeff =−46.3◦C, Komhyr et al. (1993). In the real condition each instrument has its slit function somewhat different. Thus the selected wavelengths and corresponding values of α cannot be guaranteed to be the same for all instruments. As the ozone absorption coefficients are TOeff dependant this could be the cause of different dependency of Dobson total ozone measurements on TOeff.

Komhyr, W. D., Mateer, C. L., and Hudson, R. D.: Effective BassPaur 1985 Ozone Absorption Coefficients for Use with Dobson Ozone Spectrophotometers, J. Geophys. Res., D11(98), 20 451–20 465, 1993

7.2 Smoothing error

Is an error source "smoothing error" included in the uncertainty calculation? If so, what do you define as "smoothing error"? Should the averaging kernel of the data product be applied in some way, before the uncertainty can be properly interpreted?

Answer: No.

7.3 Noise

Is there a noise contribution? If so, what do you define as "noise"? (E.g., for MOPITT, one considers an instrumental noise, but also a "geophysical noise" (Deeter, 2013).)

Answer: Precision of measurement, see Section 5.1

7.4 Random and systematic contributions

Do you consider explicitly separately "random", "structured random" and "systematic" contributions? If so, how do you define each of these in your calculation?

Answer: This information is currently assessed. It will be available in October 2017 and can be requested from the ATMOZ website (http://projects.pmodwrc.ch/atmoz/).

7.5 Input quantities / other parameters

If the main measured quantities of the data product depend on input quantities, how do the final uncertainties depend on uncertainties of these input quantities? Please provide a list with input quantities of which the uncertainties:

1. *Are taken into account.*
2. *Could be important, but are not taken into account. For example, because their consideration would be technically difficult, or it is not clear how to estimate the associated uncertainty.*
3. *Are not taken into account, as they can be demonstrated to be negligible.*

If this list is already available somewhere in a literature source, you can simply refer to it.

The impact on the measurement uncertainty due to input parameters is currently assessed and will be available in October 2017 and can be requested from the ATMOZ website (http://projects.pmodwrc.ch/atmoz/).

7.6 Uncertainty due to model error

Do you consider explicitly an uncertainty contribution due to the fact that the model is not perfect? Such uncertainty can be revealed e.g., by comparing results of several retrieval models.

Answer: The impact on the measurement uncertainty due to model error is currently assessed and will be available in October 2017 and can be requested from the ATMOZ website (http://projects.pmodwrc.ch/atmoz/).

8. Correlations/covariances

8.1 Presence in data product

Do you provide correlations or covariances within your data product, directly relevant to the main measured quantity? If so, between which quantities?

Answer: N/A

8.2 Auto-correlation

Suppose a user has to average several measured values of your data product. E.g., they want the mean column, 100 km around the observation site, within one month. Can you give a recommendation how they can obtain the uncertainty of this mean column, starting from the uncertainties provided for the individual columns?

Answer: N/A

8.3 Correlation between main measured quantity and other quantities

Do you provide any correlation info between the main measured quantity (e.g., an ozone profile) and other quantities (e.g., a temperature profile)?

Answer: N/A

9. Bias handling introduced during processing

Biases can, at least in theory, be introduced during processing. For example by nonlinear measurement equations in combination with large uncertainties on the input quantities. Is this something you try to correct for, or report, or deal with in some other way? Or do you think this will be negligible?

Answer: Possible biases are currently not taken into account in the uncertainty budget evaluation.

10. Other remarks on data product uncertainty

Please put here any other information about the data product uncertainty that you think is important.

Annex M

GAIA-CLIM questionnaire about uncertainty in data products

GNSS – Total column water vapour

Table of Contents

1. Identification of respondent and of data product

What are your contact details?

Answer:

Kalev Rannat
Tallinn University of Technology
Estonia
Email: kalev.rannat@gmail.com

For which data product are you filling in this questionnaire?

Answer:

GNSS Total Column Water Vapour

Please provide one or more accessible sources of information that a non-expert user can refer to, to gain an understanding of the measurement technique.

Answer:

Hofmann-Wellenhof, B., H. Lichtenegger, and J. Collins, GPS Theory and Practice, Springer-Verlag, Wien, New York, pp. 326, 1992.

2. Recommended literature

*Which literature work would you recommend to understand better the measurement technique and the **general uncertainty framework** within which uncertainties of the data product are constructed. Note that for metrology, the vocabulary list of the VIM (*International Vocabulary of Metrology*) and the uncertainty framework of the GUM (Guide to expression of uncertainty) are important standards. Please provide a complete reference or doi where possible.*

Answer:

Bevis, M., S. Businger, T. A. Herring, C. Rocken, R. A. Anthes, and R. H. Ware (1992), GPS meteorology– Remote-sensing of atmospheric water vapor using the Global Positioning System, J. Geophys. Res., 97(D14), 15,787–15,801.

Dow, J.M., Neilan, R. E., and Rizos, C., The International GNSS Service in a changing landscape of Global Navigation Satellite Systems, Journal of Geodesy (2009) 83:191–198, DOI: 10.1007/s00190-008-0300-3.

Jan Kouba, A GUIDE TO USING INTERNATIONAL GNSS SERVICE (IGS) PRODUCTS, Geodetic Survey Division, Natural Resources Canada, 615 Booth Street, Ottawa, Ontario K1A 0E9

Email: kouba@geod.nrcan.gc.ca
May 2009

*More specifically, which literature works (article, ATBD, other…) would you recommend to understand better how uncertainties of **this particular data product** are conceived? Please provide a complete reference or doi where possible.*

Answer:

F. J. Immler, J. Dykema, T. Gardiner, D. N. Whiteman, P. W. Thorne, and H. Vömel, Reference Quality Upper-Air Measurements: guidance for developing GRUAN data products, Atmos. Meas. Tech., 3, 1217–1231, 2010, www.atmos-meas-tech.net/3/1217/2010/, doi:10.5194/amt-3-1217-2010

T. Ning, J. Wang, G. Elgered, G. Dick, J. Wickert, M. Bradke, M. Sommer, R. Querel, and D. Smale, The uncertainty of the atmospheric integrated water vapour estimated from GNSS observations, Atmos. Meas. Tech., 9, 79–92, 2016, www.atmos-meas-tech.net/9/79/2016/, doi:10.5194/amt-9-79-2016

Please specify also if the literature source is still up-to-date with the current data product. If not, where can a user find the information on the latest version of the data product and its uncertainties?

Answer: Yes

3. Main measured quantity (measurand)

3.1 Specification of measurand

Specify the main measured quantities (i.e., the measurands) and the associated unit of the data product, along with their field name in the data product

Example measurands with unit: Temperature [K], O3 profile [ppmv], water vapour [ppmv]

Quantity [unit]	Field name
[mm] or [kg/m2]	GNSS PW or GNSS IPW or GNSS TWC or GNSS PWV or GNSS TCWV

3.2 Measurement equation

What is the relation between the main measured quantity of the data product and input quantities? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to literature publications).

Answer:

The relationship is indirect – the GNSS receiver can detect only GNSS signal delays on the ray path between an orbiting GNSS satellite and the ground-based receiver. Those delays with satellite orbital parameters and different physical constants will be inserted to a system of navigation equations [Ref. Hoffmann-Wellenhof, 1992; J. Kouba, 2009] and processed by geodetic software. One of the final products from GNSS data processing is Zenith Total Delay (ZTD). GNSS PW is derived from GNSS signal Total Zenith Delays (ZTD) by adding atmospheric and surface meteorological constraints and processing with dedicated software. The methods and principles can be found in [Bevis et al., 1992; Dow et al., 2009; T. Ning et al., 2016].

4. Traceability and comparability

4.1 SI or community traceability

Is the measurement quantity traceable, via an unbroken chain of processing steps, to SI units or community accepted standards?

Answer: Yes

If yes, please provide references to available literature describing the traceability aspects of the measurement.

T. Ning, J. Wang, G. Elgered, G. Dick, J. Wickert, M. Bradke, M. Sommer, R. Querel, and D. Smale, The uncertainty of the atmospheric integrated water vapour estimated from GNSS observations, Atmos. Meas. Tech., 9, 79–92, 2016, www.atmos-meas-tech.net/9/79/2016/, doi:10.5194/amt-9-79-2016

If no, please describe what aspects of the measurement are not fully traceable and how this aspect is addressed in deriving the data product and its uncertainty.

However, what is referred by Ning et al., is not completely implemented until now (i.e. the impact of satellite orbital errors – radial and tangential components – is not implemented in any geodetic software). The second unresolved issue is the definition and handling of formal errors in geodetic software, resulting in ZTD uncertainty used in GNSS IPW derivation, and having the dominant effect on the GNSS PW uncertainty budget (described by Ning et al.).

4.2 Comparability

If measurements are taken at multiple sites, are efforts made to ensure sufficiently similar measurement technique approaches to ensure comparability? Please provide links to any supporting materials available such as instrument manuals / network protocols.

Answer: Yes, if the measurements are taken at multiple sites and/or processed by different geodetic software (and everything is done correct) the results are sufficiently similar.

5. Representation of the uncertainty in the data product

5.1 Uncertainty field name(s)

Which field name(s) are used in the data product to hold the uncertainty value(s) associated with the main measured quantities? Note that more than one uncertainty field name can be associated with a single quantity (e.g., one field name for the "uncertainty due to random effects" and one for the "uncertainty due to systematic effects").

Field name of uncertainty	Associated quantity
σZTD	Uncertainty of Zenith Total Delay, the value (in millimetres or meters) obtainable from GNSS-data processing as a 1σ formal error. It consists of contributions of several factors (see Ning et al., 2016, subsection 3.1).
σZHD	Uncertainty of Zenith Hydrostatic Delay, value (in millimetres or meters), ref. Ning et al., 2016, subsection 3.2.
σQ	Uncertainty of a conversion factor Q, non-dimensional value, expressed as in Ning et al., 2016, subsection 3.3.

5.2 Uncertainty form

In what form is the uncertainty per measurement represented in the data product? For example, is it:

- *A standard uncertainty (i.e., uncertainty expressed as standard deviation)*
- *A 95% coverage interval*
- *A variance-covariance matrix (if so, explain between which quantities the covariance is taken into account)*
- *A probability density function*
- *Other [please specify]*

Answer: A standard uncertainty.

6. Uncertainty calculation

6.1 Formula/procedure

What is the formula/procedure by which the uncertainty is calculated? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to one or more equations in the literature).

Answer: Ning et al. 2016, subsection 3.4, Eq. 29.

Is the uncertainty obtained by:

- *Uncertainty propagation, taking into account the uncertainties of the input quantities,*

- *Probability density function propagation,*
- *Sensitivity analysis: i.e., varying parameters and check the impact on the output quantity,*
- *Or still some other procedure?*

Answer: As described in Ning et al., 2016.

6.2 Level of approximation

In what way is the uncertainty calculation procedure an approximation?

- *Is it based on (as is common practice) a first-order Taylor approximation (see GUM, Eq. (13))*

$$u_c^2(y) = \sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i, x_j) = \sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i, x_j)$$

  which will not be exact if f is nonlinear.
- *Are correlations between input quantities neglected?*
- *Other approximations?*

Answer: There are numerous models (mostly hidden in a “black-box processing”) used for getting the components from where to derive the TCW. There are nonlinear models, for example, estimating ionospheric refraction (either 2nd or 3rd order Taylor approximation) and linear approximations (like for the mean temperature of the atmosphere, Bevis et al., 1992). All approximations contribute to the final uncertainty, but as used and tested thus far, they (the models and approximations) give satisfactory results even for high-demanding precise geodetic positioning. It should be sufficient to rely on “what we get from the black-box” as these modelling uncertainties have mostly negligible effect on ZTD uncertainty, compared to possible un-even data, signal multipath, etc.

If an approximation is involved, do you think the approximation can be a problem, or do you consider it justified?

Answer: The total uncertainty of the IWV is calculated from each one of the input variables according to the rule of uncertainty propagation for uncorrelated errors.

7. Uncertainty contributions

7.1 Prior

Is there a prior contribution? If so, is this prior based on measured data, a model, a rough guess, or something else?

Answer:

All *a-priori* noise parameterizations belong to GNSS-data processing software and setup of the software. The explanations can be found from software documentation (if any).

7.2 Smoothing error

Is an error source "smoothing error" included in the uncertainty calculation? If so, what do you define as "smoothing error"? Should the averaging kernel of the data product be applied in some way, before the uncertainty can be properly interpreted?

Answer: No

7.3 Noise

Is there a noise contribution? If so, what do you define as "noise"? (E.g., for MOPITT, one considers an instrumental noise, but also a "geophysical noise" (Deeter, 2013).)

Answer:
For GNSS PW: Noise in GNSS instruments and surface meteorological parameters can be caused by thermal noise, electromagnetic interference, magnetic storms (the Sun activity), atmospheric turbulence, seismologic events etc.

7.4 Random and systematic contributions

Do you consider explicitly separately "random", "structured random" and "systematic" contributions? If so, how do you define each of these in your calculation?

Answer:
Mostly the noise has random character. However, systematic biases can be caused by instrumental changes, earthquakes etc. There exist also seasonal effects, mostly detectable while comparing the results between the summer and winter months.

7.5 Input quantities / other parameters

If the main measured quantities of the data product depend on input quantities, how do the final uncertainties depend on uncertainties of these input quantities? Please provide a list with input quantities of which the uncertainties:

1. *Are taken into account.*
2. *Could be important, but are not taken into account. For example, because their consideration would be technically difficult, or it is not clear how to estimate the associated uncertainty.*
3. *Are not taken into account, as they can be demonstrated to be negligible.*

If this list is already available somewhere in a literature source, you can simply refer to it.

Answer: Ning et al. 2016, table 4.

7.6 Uncertainty due to model error

Do you consider explicitly an uncertainty contribution due to the fact that the model is not perfect? Such uncertainty can be revealed e.g., by comparing results of several retrieval models.

Answer:
Using different models and approximation formulae in GNSS data processing is common practice and depends upon the software used and the Analysis Centre (AC) performing the calculations. No model is perfect, but if the experimental setup is correct and data reliable, then the final results from different ACs processed with different software are generally very similar.

To evaluate the results from GNSS-processing (including the models) we need independent methods applied to the data obtained from the same site at the same time. As mentioned in Ning et al. 2016, if there are at least three co-located techniques available, measuring the variability of the IWV at the same time, then a statistical analysis could be applied. However, this kind of statistical analysis is difficult to apply because three independent methods for IWV measurement are (in general) not available.

8. Correlations/covariances

8.1 Presence in data product

Do you provide correlations or covariances within your data product, directly relevant to the main measured quantity? If so, between which quantities?

Answer: No

8.2 Auto-correlation

Suppose a user has to average several measured values of your data product. E.g., they want the mean column, 100 km around the observation site, within one month. Can you give a recommendation how they can obtain the uncertainty of this mean column, starting from the uncertainties provided for the individual columns?

Answer:
For GNSS PW, this is mostly impossible due to the low density of GNSS-sites. Just calculating the mean column for a certain time period for one site is trivial, but the uncertainty calculation must follow the methodology explained in Ning et al., 2016.

8.3 Correlation between main measured quantity and other quantities

Do you provide any correlation info between the main measured quantity (e.g., an ozone profile) and other quantities (e.g., a temperature profile)?

Answer: No, but it could be done.

9. Bias handling introduced during processing

Biases can, at least in theory, be introduced during processing. For example by nonlinear measurement equations in combination with large uncertainties on the input quantities. Is this something you try to correct for, or report, or deal with in some other way? Or do you think this will be negligible?

Answer: Yes, the bias can be detected, but only afterwards while analysing the time series and comparing with independent measurements.

10. Other remarks on data product uncertainty

Please put here any other information about the data product uncertainty that you think is important.

Annex N

GAIA-CLIM questionnaire about uncertainty in data products

GRUAN radiosondes – Temperature & humidity profiles

Table of Contents

1. Identification of respondent and of data product

What are your contact details?

Answer:
Peter Thorne
Maynooth University Department of Geography
Maynooth
Co. Kildare
Ireland
M: +353 87 612 2753
E: peter.thorne@nuim.ie
W: www.maynoothuniversity.ie/geography

For which data product are you filling in this questionnaire?

Answer: GRUAN RS92 radiosonde product

Please provide one or more accessible sources of information that a non-expert user can refer to, to gain an understanding of the measurement technique.

Answer:
http://www.vaisala.com/en/products/soundingsystemsandradiosondes/radiosondes/Pages/RS92.aspx provides the manufacturer based instrument specification.

https://www.wmo.int/pages/prog/www/IMOP/publications/CIMO-Guide/Provis2014Ed/Provisional2014Ed_P-I_Ch-12.pdf provides the description of radiosonde techniques more generally in the CIMO Guide to measurements.

2. Recommended literature

Which literature work would you recommend to understand better the measurement technique and the ***general uncertainty framework*** *within which uncertainties of the data product are constructed. Note that for metrology, the vocabulary list of the VIM (*International Vocabulary of Metrology*), and the uncertainty framework of the GUM (Guide to expression of uncertainty) are important standards. Please provide a complete reference or doi where possible.*

Answer:
The GRUAN data product undertakes a full metrological characterisation based upon lab, bench and field characterisation of the instrument. The analysis is traceable and the analysis is

commensurate with the GUM practices and the VIM. The GRUAN measurement framework is given in:

F. J. Immler, J. Dykema, T. Gardiner, D. N. Whiteman, P. W. Thorne, and H. Vömel, Reference Quality Upper-Air Measurements: guidance for developing GRUAN data products, Atmos. Meas. Tech., 3, 1217-1231, 2010 http://www.atmos-meas-tech.net/3/1217/2010/doi:10.5194/amt-3-1217-2010

The specific data processing and characterisation undertaken in the v2 data product is given in:

R. J. Dirksen, M. Sommer, F. J. Immler, D. F. Hurst, R. Kivi, and H. Vömel, Reference quality upper-air measurements: GRUAN data processing for the Vaisala RS92 radiosonde, Atmos. Meas. Tech., 7, 4463-4490, 2014 http://www.atmos-meas-tech.net/7/4463/2014/doi:10.5194/amt-7-4463-2014

More specifically, which literature works (article, ATBD, other…) would you recommend to understand better how uncertainties of ***this particular data product*** *are conceived? Please provide a complete reference or doi where possible.*

Answer:
A GRUAN Technical Document (equivalent to ATBD) is in preparation but not available at the time of writing. The Vaisala RS92 manufacturer page provides a manufacturer claimed set of performances and a description on techniques. This is available at http://www.vaisala.com/en/products/soundingsystemsandradiosondes/radiosondes/Pages/RS92.aspx . Note, however, that the GRUAN processing includes a set of additional processing steps as described in Dirksen et al. The Dirksen et al paper describes the full uncertainty derivation. References therein provide additional pioneering efforts at instrument characterisation that it builds upon.

Also useful are the series of CIMO intercomparison campaigns which compare over an intensive field campaign a large number of radiosonde models. The most recent such comparison was held at Yangjiang, China and involved the RS92 instrument. The results can be found at: https://www.wmo.int/pages/prog/www/IMOP/publications/IOM-107_Yangjiang.pdf

Please specify also if the literature source is still up-to-date with the current data product. If not, where can a user find the information on the latest version of the data product and its uncertainties?

Answer:
Dirksen et al. provides the description for the version 2 product made available publically. A version 3 product is under development that incorporates new instrument understanding. It remains unclear how GRUAN shall chose to document v3 upon release, but it shall be documented.

3. Main measured quantity (measurand)

3.1 Specification of measurand

Specify the main measured quantities (i.e., the measurands) and the associated unit of the data product, along with their field name in the data product

Example measurands with unit: Temperature [K], O3 profile [ppmv], water vapour [ppmv]

Quantity [unit]	Field description	Field name
K	Air temperature	Temp
hPa	Air pressure	Press
%RH	Relative humidity	Rh
Degrees	Wind direction	Wdir
$m.s^{-1}$	Wind speed	Wspeed
m	Geopotential height	Geopot
Ppmv	Water vapour mixing ratio	WVMR
K	Frostpoint	FP

Note the above is a sub-sample of principal measurements information retained in the comprehensive netcdf files. See files at e.g. ftp://ftp.ncdc.noaa.gov/pub/data/gruan/processing/level2/RS92-GDP/version-002/LIN/2016/ for a sample of the measurement series, variables and uncertainty information provided. Principal uncertainties are on the air temperature and water vapour related variables.
The GRUAN data product for RS92 is described in GRUAN Technical Document 4, Brief description of the RS92 GRUAN Data Product (RS92-GDP)
http://www.dwd.de/EN/research/international_programme/gruan/download/gruan_td-4.pdf?__blob=publicationFile&v=4

3.2 Measurement equation

What is the relation between the main measured quantity of the data product and input quantities? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to literature publications).

Answer:
Although never formally derived in the form of a measurement equation, the relevant measurement equation components are outlined and fully described in Dirksen et al., 2014. There are distinct equations required for each of the reporting elements. The GRUAN product processing is primarily concerned with the temperature and humidity instruments.

The temperature sensor characterisation and processing is described in Section 5 of Dirksen et al.

The humidity sensor characterisation and processing is described in Section 6 of Dirksen et al.

Derived measurement quantities are dependent upon the *implicit* measurement equations associated with each of the primary instruments.

4. Traceability and comparability

4.1 SI or community traceability

Is the measurement quantity traceable, via an unbroken chain of processing steps, to SI units or community accepted standards?

Answer: Yes.

If yes, please provide references to available literature describing the traceability aspects of the measurement.

The characterisation of the instrument is fully described in Dirksen et al., 2014 reference given above which details a suite of chamber, bench and environmental tests and comparisons to build confidence in the resulting estimates.

If no, please describe what aspects of the measurement are not fully traceable and how this aspect is addressed in deriving the data product and its uncertainty.

4.2 Comparability

If measurements are taken at multiple sites, are efforts made to ensure sufficiently similar measurement technique approaches to ensure comparability? Please provide links to any supporting materials available such as instrument manuals / network protocols.

Answer:
Yes, the data are collected using consistent ground-based pre-launch calibrations. The calibration data and the raw digital count data files in their instrument-to-ground-segment transmitted form are collated and stored at the GRUAN lead centre using a common web-based collection client (RSlaunchclient) that also collects necessary additional metadata. All received raw data files are reprocessed using a single processing algorithm that performs processing in a consistent manner across the network and provides output in an identical repeating format both over time and between sites. On version increments the entire series is reprocessed to yield a long-term consistent series.

5. Representation of the uncertainty in the data product

5.1 Uncertainty field name(s)

Which field name(s) are used in the data product to hold the uncertainty value(s) associated with the main measured quantities? Note that more than one uncertainty field name can be associated with a single quantity (e.g., one field name for the "uncertainty due to random effects" and one for the "uncertainty due to systematic effects").

Uncertainty description	Associated quantity	Field name
Air temperature correlated uncertainty	Air temperature	U_cor_temp

Air temperature standard deviation	Air temperature	U_std_temp
Air temperature total uncertainty	Air temperature	U_temp
Relative humidity standard deviation	Relative humidity	U_std_rh
Relative humidity correlated uncertainty	Relative humidity	U_cor_rh
Relative humidity total uncertainty	Relative humidity	U_rh
Wind speed uncorrelated uncertainty	Wind speed	U_wspeed
Wind direction uncorrelated uncertainty	Wind direction	U_wdir
Pressure total uncertainty	Pressure	U_press
Altitude total uncertainty	Geometric altitude	U_alt

See GRUAN Technical Document 4 for a description of the uncertainty fields.

http://www.dwd.de/EN/research/international_programme/gruan/download/gruan_td-4.pdf?__blob=publicationFile&v=4

5.2 Uncertainty form

In what form is the uncertainty per measurement represented in the data product? For example, is it:

- *A standard uncertainty (i.e., uncertainty expressed as standard deviation)*
- *A 95% coverage interval*
- *A variance-covariance matrix (if so, explain between which quantities the covariance is taken into account)*
- *A probability density function*
- *Other [please specify]*

Answer:
Standard uncertainty. Within the files the reported values are 1-sigma ranges.

6. Uncertainty calculation

6.1 Formula/procedure

What is the formula/procedure by which the uncertainty is calculated? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to one or more equations in the literature).

Answer:
The uncertainty calculation is discussed in Dirksen et al., 2014 for each of the principal measurement series. Typically there are several sources of uncertainty quantified for each measured parameter via a range of lab, bench and field comparison techniques. Each of these sources of uncertainty is derived experimentally and parameterised mathematically as described

in Dirksen et al., 2014. For all measurements there exists a calibration uncertainty which is a perfectly correlated term within each measurement series profile.

For temperature measurements the uncertainty arises from:

- Absolute uncertainty of T sensor calibration
- Random uncertainty
- Radiation related terms:
    - Uncertainty due to sonde rotation
    - Uncertainty due to uncertainty in albedo
    - Uncertainty due to ventilation (ascent rate) uncertainty
    - Uncertainty due to uncertainty in radiative correction model fit terms

See Dirksen et al., Table 2 and associated discussion in Section 5.

For humidity measurements primary reported variable, RH, the uncertainty arises from:

- Calibration uncertainty
- Uncertainty in the temperature dependent calibration corrections
- Uncertainty in time lag corrections
- Uncertainty in the radiation dry bias corrections
- Random uncertainty term

See Dirksen et al, Table 6 and associated discussion in Section 6.

Is the uncertainty obtained by:

- *Uncertainty propagation, taking into account the uncertainties of the input quantities,*
- *Probability density function propagation,*
- *Sensitivity analysis: i.e., varying parameters and check the impact on the output quantity,*
- *Or still some other procedure?*

Answer:
Uncertainty propagation. In general different sources of uncertainty are considered to be independent so final estimates consist of an estimate that results from their combination in quadrature. In the v2 product for those terms where the uncertainty has not been calculated explicitly to account for any identified co-dependencies, the co-dependencies are not modelled.

The envisaged version 3 product will provide a breakdown in some appropriate combination of random, structured random and systematic components.

6.2 Level of approximation

In what way is the uncertainty calculation procedure an approximation?

- *Is it based on (as is common practice) a first-order Taylor approximation (see GUM, Eq. (13))*

$$u_c^2(y) = \sum_{i=1}^{N}\sum_{j=1}^{N} \frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j} u(x_i, x_j) = \sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N} \frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j} u(x_i, x_j)$$

which will not be exact if f is nonlinear.

- *Are correlations between input quantities neglected?*
- *Other approximations?*

Answer:
The true actinic flux, particularly above the first cloud layer cannot be known as the subsequent cloud structure is unknown so approximations to the radiation effects are required in creating the best estimate for both temperature and RH and potentially result in incorrect uncertainty estimates compared to if the true actinic flux were known for each profile.

For the temperature measurements spike removal and sensor time lag which are minor systematic effects are excluded because there is no rigorous way to quantify them. The random term is commensurately inflated.

Correlations between sources of uncertainty are neglected in the v2 product in the vast majority of cases.

If an approximation is involved, do you think the approximation can be a problem, or do you consider it justified?

Answer:
The approximation regarding flux results may yield an under-estimation of temperature uncertainty in some cases (implied from Dirksen et al., Figure 10). The assumption of independence of uncertainty sources may potentially lead to issues of under-estimating the vertical persistence of certain uncertainties within a given radiosonde measured profile if the uncertainty terms are treated naively by the end-user.

7. Uncertainty contributions

7.1 Prior

Is there a prior contribution? If so, is this prior based on measured data, a model, a rough guess, or something else?

Answer: The calibration uncertainty provides a prior term that is known and is correlated throughout the profile.

The pendulum effect is a prior based upon physical first principals determined from harmonic frequencies but its phasing is unknown.

The humidity sensor dry bias and time lag correction terms are based upon prior terms determined through lab testing and in the field comparisons.

The actinic flux prior is determined by lab tests, and its value for a given location, date and time determined by the time of year, location and time of day and differences between the prescribed flux and the (unknown) real-world flux, which is a function of cloud and particulate structure.

7.2 Smoothing error

Is an error source "smoothing error" included in the uncertainty calculation? If so, what do you define as "smoothing error"? Should the averaging kernel of the data product be applied in some way, before the uncertainty can be properly interpreted?

Answer:
For the humidity measurements the instrument response time at cold temperatures leads to an overly smooth profile (termed time lag) which constitutes a smoothing error, and is overcome by inferring structure through a statistical inversion technique, which has an associated uncertainty that is quantified.

7.3 Noise

Is there a noise contribution? If so, what do you define as "noise"? (E.g., for MOPITT, one considers an instrumental noise, but also a "geophysical noise" (Deeter, 2013).)

Answer:
Both the temperature and humidity sensor measurements include a random measurement uncertainty term that includes instrument-to-instrument noise and unaccounted for minor effects and has been verified through dual-launch soundings.

7.4 Random and systematic contributions

Do you consider explicitly separately "random", "structured random" and "systematic" contributions? If so, how do you define each of these in your calculation?

Answer:
Random and perfectly correlated systematic uncertainties are reported for some parameters in the v2 product.

Some parameters reported as random are in-fact structured random. For example, the effects of pendulum swinging is a known function of the string length, so shall have a known periodicity. Uncertainties that are dependent upon the instrument direction at a given time will have a periodicity that matches that of the pendulum resonant frequency. Currently such terms are treated as random but are clearly structured random such that effects at the frequency of the effect shall be highly correlated.

7.5 Input quantities / other parameters

If the main measured quantities of the data product depend on input quantities, how do the final uncertainties depend on uncertainties of these input quantities? Please provide a list with input quantities of which the uncertainties:

1. *Are taken into account.*
2. *Could be important, but are not taken into account. For example, because their consideration would be technically difficult, or it is not clear how to estimate the associated uncertainty.*
3. *Are not taken into account, as they can be demonstrated to be negligible.*

If this list is already available somewhere in a literature source, you can simply refer to it.

The full list is given in the text and various tables of Dirksen et al., 2014.

7.6 Uncertainty due to model error

Do you consider explicitly an uncertainty contribution due to the fact that the model is not perfect? Such uncertainty can be revealed e.g., by comparing results of several retrieval models.

Answer: Implicit in the actinic flux corrections which depend upon RT modelling assumptions.

8. Correlations/covariances

8.1 Presence in data product

Do you provide correlations or covariances within your data product, directly relevant to the main measured quantity? If so, between which quantities?

Answer: Not in the present v2 product. Some consideration of such effects is to be achieved in the v3 product.

8.2 Auto-correlation

Suppose a user has to average several measured values of your data product. E.g., they want the mean column, 100 km around the observation site, within one month. Can you give a recommendation how they can obtain the uncertainty of this mean column, starting from the uncertainties provided for the individual columns?

Answer:
Aspects of this were explicitly considered within Bodeker and Kremser, 2015

G. E. Bodeker and S. Kremser, Techniques for analyses of trends in GRUAN data, Atmos. Meas. Tech., 8, 1673–1684, 2015, www.atmos-meas-tech.net/8/1673/2015/doi:10.5194/amt-8-1673-2015.

This publication considers primarily questions around the effects of uncertainty quantification on trend determination although also touches on other aspects of averaging samples appropriately.

8.3 Correlation between main measured quantity and other quantities

Do you provide any correlation info between the main measured quantity (e.g., an ozone profile) and other quantities (e.g., a temperature profile)?

Answer:
Dependencies of the humidity measurement on temperatures are explicitly included. There is some dependency of temperature on humidity upon emergence from cloud when the temperature sensor temporarily acts as a wet bulb. This is minimal, but shall affect small segments of the profile and is not directly modelled. There are also correlations between WVMR and pressure, and pressure and geopotential height. The pressure-GPH connection stems from the fact that pressure and GPS data are combined to calculate pressure and (geo)potential profiles that are mutually consistent.

9. Bias handling introduced during processing

Biases can, at least in theory, be introduced during processing. For example by nonlinear measurement equations in combination with large uncertainties on the input quantities. Is this something you try to correct for, or report, or deal with in some other way? Or do you think this will be negligible?

Answer:
The uncertainties related to all steps in the processing have been identified and quantified. These uncertainties include any potential mis-specifications of the removed systematic uncertainties during the processing. Redundant dual launches and launches coincident with additional measurement techniques build confidence that no large biases remain through most of the profile. A potential temperature bias at the very highest levels has been identified and shall be addressed in the v3 product. In version 2 the SHC groundcheck data at 100 %RH are not used to correct the humidity profiles, although this is foreseen for v3.

10. Other remarks on data product uncertainty

Please put here any other information about the data product uncertainty that you think is important.

Annex O

GAIA-CLIM questionnaire about uncertainty in data products

GRUAN – Top-of-atmosphere brightness temperatures

Table of Contents

1. Identification of respondent and of data product

What are your contact details?

Answer:
Dr William Bell
Satellite Applications, Weather Science
Met Office
FitzRoy Road
Exeter
EX1 3PB
Devon
United Kingdom
Email: william.bell@metoffice.gov.uk

For which data product are you filling in this questionnaire?

Answer: Top-of-atmosphere (TOA) brightness temperatures simulated from GRUAN radiosonde measurements *and* NWP models, in order to provide estimates of the uncertainties in simulations based on NWP models (here the working assumption is that the GRUAN measurements provide a *proxy* for truth).

Please provide one or more accessible sources of information that a non-expert user can refer to, to gain an understanding of the measurement technique.

Answer: The approach being developed in GAIA-CLIM WP4, establishing the uncertainties in simulated TOA brightness temperatures generated from NWP models, is novel. However, work has been done recently to validate retrievals ('Level 2') using GRUAN data (Reale *et al* (2012)). In addition, the use of NWP-based simulations to validate satellite brightness temperature measurements ('Level 1') is well established (Bell *et al* (2008) , Lu *et al* (2011), Bormann *et al* (2013)).

W. Bell, S. English, B. Candy, N. Atkinson, F. Hilton, S. Swadley, W. Campbell, N. Bormann, G. Kelly and M. Kazumori, The Assimilation of SSMIS Radiances in Numerical Weather Prediction Models, *IEEE Transactions on Geoscience and Remote Sensing, Vol 45, April 2008.*

Qifeng Lu, W. Bell, P. Bauer, N. Bormann and C. Peubey, Characterising the FY-3A Microwave Temperature Sounder Using the ECMWF Model, *Journal of Oceanic and Atmospheric Technology*, Volume 28, Issue 11 (November 2011) pp. 1373-,1389, doi: 10.1175/JTECH-D-10-05008.1.

Niels Bormann, Anne Fouilloux and William Bell, Evaluation and assimilation of ATMS data in the ECMWF system, Geophys. Res Lett, 2013.

Tony Reale, Bomin Sun, Franklin H. Tilley, Michael Pettey, The NOAA Products Validation System (NPROVS) Journal of Atmospheric and Oceanic Technology, May 2012, Vol. 29, No. 5, 1 May 2012.

2. Recommended literature

*Which literature work would you recommend to understand better the measurement technique and the **general uncertainty framework** within which uncertainties of the data product are constructed. Note that for metrology, the vocabulary list of the VIM (*International Vocabulary of Metrology*) and the uncertainty framework of the GUM (Guide to expression of uncertainty) are important standards. Please provide a complete reference or doi where possible.*

Answer:

Immler, F. J., and M. Sommer, 2011: Brief description of the RS92 GRUAN data product (RS92-GDP). Revision 1.1, GRUAN Tech. Doc. GRUAN-TD-4, 17 pp. [Available online at http://www.dwd.de/bvbw/generator/DWDWWW/Content/Projekte/Gruan/Downloads/documents/gruan-td-4,templateId=raw,property=publicationFile.pdf/gruan-td-4.pdf .]

Dirksen, R. J., M. Sommer, F. J. Immler, D. F. Hurst, R. Kivi, and H. Vömel, 2014: Reference quality upper-air measurements: GRUAN data processing for the Vaisala RS92 radiosonde. Atmos. Meas. Tech. Discuss.,7,3727–3800, doi:10.5194/amtd-7-3727-2014.

*More specifically, which literature works (article, ATBD, other…) would you recommend to understand better how uncertainties of **this particular data product** are conceived? Please provide a complete reference or doi where possible.*

Answer: The projection of the specified uncertainties in the GRUAN radiosonde profile product to TOA brightness temperature uncertainties is the subject of ongoing work as part of the GAIA-CLIM project. There is, as yet, no publication describing the methods under development. It is anticipated that such a publication will be produced as an output of the GAIA-CLIM project.

Tech-memo available on gaia-clim website http://www.gaia-clim.eu/biblio/introduction-gruan-processor

Please specify also if the literature source is still up-to-date with the current data product. If not, where can a user find the information on the latest version of the data product and its uncertainties?

Answer: N/A

3. Main measured quantity (measurand)

3.1 Specification of measurand

Specify the main measured quantities (i.e., the measurands) and the associated unit of the data product, along with their field name in the data product

Example measurands with unit: Temperature [K], O3 profile [ppmv], water vapour [ppmv]

Quantity [unit]	Field name
(Simulated) TOA brightness temperatures (K)	Brightness temperatures simulated from (i) GRUAN radiosonde profiles; or (ii) NWP model fields

3.2 Measurement equation

What is the relation between the main measured quantity of the data product and input quantities? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to literature publications).

Answer:

$$\hat{y} = H(\hat{x})$$

where :

$\hat{y}$ is a vector of simulated radiances (with the elements of the vector representing the brightness temperatures for individual channels of a radiometer) and

$\hat{x}$ is a state vector containing a profile of atmospheric temperature, humidity and surface parameters required for the observation operator (H).

H is an observation operator which maps the atmospheric state vector to a vector of TOA brightness temperatures for a given instrument. In this case the observation operator takes the form of a fast radiative transfer model (RTTOV) – which is a parametrised version of a full line-by-line radiative transfer model.

4. Traceability and comparability

4.1 SI or community traceability

Is the measurement quantity traceable, via an unbroken chain of processing steps, to SI units or community accepted standards?

Answer: Although the GRUAN measurements themselves are traceable (Dirksen (2014)), the radiative transfer model which projects these into TOA brightness temperatures is based on spectroscopic parameters (linestrength, linewidths, and pressure broadening parameters) that are not traceable.

If yes, please provide references to available literature describing the traceability aspects of the measurement.

Dirksen, R. J., M. Sommer, F. J. Immler, D. F. Hurst, R. Kivi, and H. Vömel, 2014: Reference quality upper-air measurements: GRUAN data processing for the Vaisala RS92 radiosonde. Atmos. Meas. Tech. Discuss.,7, 3727–3800, doi:10.5194/amtd-7-3727-2014.

If no, please describe what aspects of the measurement are not fully traceable and how this aspect is addressed in deriving the data product and its uncertainty.

In this data product, uncertainties in the NWP simulated brightness temperatures are estimated from differences between NWP based simulations and GRUAN simulations. The errors introduced by the RT modelling are therefore to first order cancelled, leaving the main contribution from the differences between GRUAN and NWP, expressed as TOA brightness temperatures.

4.2 Comparability

If measurements are taken at multiple sites, are efforts made to ensure sufficiently similar measurement technique approaches to ensure comparability? Please provide links to any supporting materials available such as instrument manuals / network protocols.

Answer: The method is applied to observations from all GRUAN sites.

5. Representation of the uncertainty in the data product

5.1 Uncertainty field name(s)

Which field name(s) are used in the data product to hold the uncertainty value(s) associated with the main measured quantities? Note that more than one uncertainty field name can be associated with a single quantity (e.g., one field name for the "uncertainty due to random effects" and one for the "uncertainty due to systematic effects").

Product still under development.

Field name of uncertainty	Associated quantity
u_total_bt	Total uncertainty on BT

5.2 Uncertainty form

In what form is the uncertainty per measurement represented in the data product? For example, is it:

- *A standard uncertainty (i.e., uncertainty expressed as standard deviation)*
- *A 95% coverage interval*
- *A variance-covariance matrix (if so, explain between which quantities the covariance is taken into account)*
- *A probability density function*
- *Other [please specify]*

Answer: Product still under development.

6. Uncertainty calculation

6.1 Formula/procedure

What is the formula/procedure by which the uncertainty is calculated? (You can use the equation editor, or paste a snapshot of the formula, or simply refer to one or more equations in the literature).

Answer: TBD. Product still under development. See Dirksen et al. 2014 for GRUAN uncertainties.

Is the uncertainty obtained by:

- *Uncertainty propagation, taking into account the uncertainties of the input quantities,*
- *Probability density function propagation,*
- *Sensitivity analysis: i.e., varying parameters and check the impact on the output quantity,*
- *Or still some other procedure?*

Answer: Probability density function propagation.

6.2 Level of approximation

In what way is the uncertainty calculation procedure an approximation?

- *Is it based on (as is common practice) a first-order Taylor approximation (see GUM, Eq. (13))*

$$u_c^2(y) = \sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i, x_j) = \sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}u(x_i, x_j)$$

which will not be exact if f is nonlinear.

- *Are correlations between input quantities neglected?*
- *Other approximations?*

Answer: An approximation is made that RT modelling differences, arising from uncertainties in spectroscopic parameters, and discretisation of a full line-by-line RT calculation, cancel when differences are taken between NWP simulated and GRUAN simulated profiles.

If an approximation is involved, do you think the approximation can be a problem, or do you consider it justified?

Answer: As a working hypothesis, the approximation is assumed valid. Further development of the product, and evaluation, will shed light on whether this approximation is valid.

7. Uncertainty contributions

7.1 Prior

Is there a prior contribution? If so, is this prior based on measured data, a model, a rough guess, or something else?

Answer: No. The 'forward calculation' involved in generating level 1 brightness temperatures, is free from any dependence on a prior.

7.2 Smoothing error

Is an error source "smoothing error" included in the uncertainty calculation? If so, what do you define as "smoothing error"? Should the averaging kernel of the data product be applied in some way, before the uncertainty can be properly interpreted?

Answer: No.

7.3 Noise

Is there a noise contribution? If so, what do you define as "noise"? (E.g., for MOPITT, one considers an instrumental noise, but also a "geophysical noise" (Deeter, 2013).)

Answer: N/A.

7.4 Random and systematic contributions

Do you consider explicitly separately "random", "structured random" and "systematic" contributions? If so, how do you define each of these in your calculation?

Answer: TBD. Product still under development.

7.5 Input quantities / other parameters

If the main measured quantities of the data product depend on input quantities, how do the final uncertainties depend on uncertainties of these input quantities? Please provide a list with input quantities of which the uncertainties:

1. *Are taken into account.*
2. *Could be important, but are not taken into account. For example, because their consideration would be technically difficult, or it is not clear how to estimate the associated uncertainty.*
3. *Are not taken into account, as they can be demonstrated to be negligible.*

If this list is already available somewhere in a literature source, you can simply refer to it.

Input quantity/other parameter	associated uncertainty or "important but ignored" or "negligible"	Extra info (e.g., random, systematic)
GRUAN temperature profile	Taken into account	Random & systematic
GRUAN pressure profile	Taken into account	Random & systematic
GRUAN humidity profile	Taken into account	Random & systematic
Surface pressure, temperature and humidity.	Taken into account	Random & systematic
NWP equivalents of above.	Taken into account	Random

7.6 Uncertainty due to model error

Do you consider explicitly an uncertainty contribution due to the fact that the model is not perfect? Such uncertainty can be revealed e.g., by comparing results of several retrieval models.

Answer: N/A.

8. Correlations/covariances

8.1 Presence in data product

Do you provide correlations or covariances within your data product, directly relevant to the main measured quantity? If so, between which quantities?

Answer: Still under development. Requires specified correlations in input quantities (GRUAN profiles) which are themselves still under development.

8.2 Auto-correlation

Suppose a user has to average several measured values of your data product. E.g., they want the mean column, 100 km around the observation site, within one month. Can you give a recommendation how they can obtain the uncertainty of this mean column, starting from the uncertainties provided for the individual columns?

Answer: N/A

8.3 Correlation between main measured quantity and other quantities

Do you provide any correlation info between the main measured quantity (e.g., an ozone profile) and other quantities (e.g., a temperature profile)?

Answer: N/A

9. Bias handling introduced during processing

Biases can, at least in theory, be introduced during processing. For example by nonlinear measurement equations in combination with large uncertainties on the input quantities. Is this something you try to correct for, or report, or deal with in some other way? Or do you think this will be negligible?

Answer: TBD

10. Other remarks on data product uncertainty

Please put here any other information about the data product uncertainty that you think is important.