Annex C

GAIA-CLIM questionnaire about uncertainty in data products

Lidar – Ozone profiles

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1. Identification of respondent and of data product

What are your contact details?

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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. Schönenborn, I. S. McDermid, T. Leblanc, S. Godin, T. Song, D. P. J. Swart, Y. J. Meijer, G. E. Bodeker, B. J. Connor, N. Kämpfer, K. Hocke, Y. Calisesi, N. Schneider, J. de la Noë, A. D. Parrish, I. S. Boyd, C. Brühl, 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.