# Standardized Definition and Reporting of Vertical Resolution and Uncertainty in the NDACC Lidar Ozone and Temperature Algorithms.

## Summary

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## Motivation

As part of the Network for Detection of Stratospheric Change (NDACC), over 20 ground-based lidar instruments are dedicated to the long-term monitoring of atmospheric composition and to the validation of space-borne measurements of Earth's atmosphere from environmental satellites (e.g., EOS-Aura, ENVISAT, NPP, Sentinel). In networks such as NDACC, the instruments use a wide spectrum of methodologies and technologies to measure key atmospheric parameters such as ozone, temperature, water vapor, etc. One ensuing caveat is the difficulty to archive measurement and analysis information consistently within all research groups (or instruments). Yet the need for consistent definitions has strengthened as datasets of various origin (e.g., satellite and ground-based) need increased quality control and thorough validation before they can be used for long-term trend studies or be ingested together in global assimilation systems. Within the NDACC Lidar Working Group, a few studies for example have shown the impact on ozone of using different definitions of vertical resolution (e.g., Beyerle and McDermid, 1999; Godin-Beekmann et al., 1999), or have estimated the impact of various corrections on temperature (e.g., Leblanc et al., 1998), but little work was done to facilitate a standardization of the definitions and approaches relating to vertical resolution and uncertainty budget.

In order to address such need for consistency within NDACC lidar data, several NDACC lidar collaborators have joined forces through the formation in 2011 of an *International Space Science Institute* (ISSI) International Team of Experts (http://www.issibern.ch/aboutissi/mission.html). The objective of this working group (henceforth "ISSI Team") was to provide scientifically meaningful recommendations for the use of standardized definitions of vertical resolution and standardized definitions and approaches for the treatment of uncertainty in the NDACC ozone and temperature lidar retrievals. Ultimately, the recommendations were designed so that they can be implemented consistently by all NDACC ozone and temperature lidar investigators.

The ISSI Team Report comprises two distinct parts. Part 1 is exclusively dedicated to vertical resolution while Part 2 is exclusively dedicated to uncertainties. The treatment of uncertainty is significantly more complex than that of vertical resolution. As a result, Part 2 is significantly longer than Part 1. It is organized in six "chapters" and complemented by ten appendices, while Part 1 comprises only four sections. Though the focus is on the retrieval of ozone by the differential absorption technique and temperature by the density integration technique, many concepts described in the report can be applied to the retrieval of other NDACC species such as water vapor (Raman and differential absorption techniques), temperature (rotational Raman technique), and aerosol backscatter ratio. Supplements to the present report on these topics are expected in the coming years. The present summary outlines the main results detailed in Part 1 and Part 2, and briefly reviews how the ISSI Team recommendations may be implemented within NDACC in the upcoming months or years.

# 1 Standardized definitions of vertical resolution

Generally speaking, vertical resolution, as provided by the lidar investigators in the archived NDACC data files, is an indicator of the amount of vertical filtering applied to the lidar signals or to the species profiles. This filtering is applied in order to reduce high frequency noise typically produced at the signal detection level. Because the signal-to-noise ratio varies with altitude, the amount of applied filtering usually depends on altitude, with more filtering being applied at higher altitudes. Over the years, NDACC lidar PIs have been providing temperature and ozone profiles using a wide range of vertical resolution schemes and values. The definition of vertical resolution used appears to differ significantly. To address this issue, the ISSI Team reviewed the various vertical resolution schemes and definitions in use by the NDACC PIs, and agreed on the recommendation of two standardized definitions for use in future NDACC-archived data.

## 1.1 Definition based on the FWHM of a finite impulse response

Whether we consider the lidar signal or the retrieved species, vertical filtering at a specific altitude consists of a linear combination of multiple samples at the neighboring altitudes. The coefficients of the filter used in the smoothing operation are chosen by the lidar investigator, and constitute the key information for the derivation of a standardized definition of vertical resolution. The first ISSI Team "standardized" definition recommended for use in the NDACC ozone and temperature lidar algorithms is based on the width of the response to a Finite Impulse-type perturbation. The response is computed by convolving the filter coefficients with an impulse function, namely, a Kronecker Delta function for smoothing filters, and a Heaviside Step function for derivative filters. Once the response has been computed, the standardized definition of vertical resolution proposed by the ISSI Team is given by $\Delta z = \delta z * H_{FWHM}$, where $\delta z$ is the lidar's sampling resolution and $H_{FWHM}$ is the full-width at half-maximum (FWHM) of the response, measured in sampling intervals. Following this definition, an unsmoothed signal yields the best possible vertical resolution $\Delta z = \delta z$ (one sampling bin).

This definition was recommended by the ISSI Team because it is already widely used within the NDACC community, and it has many points of commonality with the averaging kernels reported for the retrieval of atmospheric species using passive techniques and optimal estimation methods. This definition also allows multiple smoothing occurrences to be treated analytically in a simple and exact manner (see paragraph 1.3).

## 1.2 Definition based on the cut-off frequency of a digital filter

The other recommended definition relates to digital filtering theory (Hamming, 1977). After applying a Laplace Transform to a set of filter coefficients, we can derive the filter's transfer function and gain, which characterize the effect of the filter on the signal in the frequency-domain. A gain value close to 1.0 at a given frequency means that the smoothing has no or very little effect at this particular frequency, while a value close to 0.0 means that this frequency component was fully suppressed by the smoothing process. A cut-off frequency value can be defined as the frequency at which the gain equals 0.5. Perturbations of this frequency see their magnitude divided by 2 after smoothing. Vertical resolution can then be defined by the relation $\Delta z = \delta z/(2f_C)$, where $f_C$ is the cut-off frequency. Unlike common practice in the field of spectral analysis, a factor $2f_C$ instead of $f_C$ is indeed proposed here because it yields values of vertical resolution that are conveniently equal, or close to the values obtained using the impulse response definition described in the previous paragraph. The present definition therefore yields vertical resolution values expressed as multiples of sampling intervals rather than multiples of Nyquist intervals, and an unsmoothed signal yields the best possible vertical resolution $\Delta z = \delta z$ (one sampling interval), corresponding in the frequency domain, to twice the Nyquist frequency.

One advantage of a definition based on cutoff frequency is that the computed values reflect the actual impact of filtering on geophysical perturbations independently of the type of filter used. Like in the impulse response case, the values of vertical resolution computed for multiple, successive smoothing operations is conceptually, theoretically and numerically exact (see next paragraph). In the case of the differential absorption lidar technique, the process of smoothing and the process of differentiating the ratio of the signals collected at the absorbed and non-absorbed wavelengths are often combined in the same filtering operation. For the resulting derivative filters, the application of the digital filter theory is similar to that of smoothing filters.

### 1.3 Practical implementation to NDACC lidars

The ISSI-Team developed numerical tools to support the implementation of this definition across the NDACC lidar groups. These tools consist of ready-to-use "plug-in" routines written in IDL, FORTRAN and MATLAB that can be inserted into the NDACC lidar PIs' data processing software each time a smoothing operation occurs in their data processing chain. The routine's input parameters are the coefficients of the smoothing filter applied to the lidar signal or to the temperature or ozone profile, and the output parameter is the vertical resolution following the impulse response-based standardized definition or the cut-off frequency-based standardized definition. The values output by the routines can then be reported in the NDACC lidar data files together with the ozone or temperature profiles.

In the impulse response definition case, the plug-in routine not only outputs the vertical resolution, but also the response itself over the full sampling interval considered. When multiple smoothing operations occur within the same data processing chain, the plug-in routine is called each time smoothing occurs, and the impulse response output by the routine during the previous smoothing occurrence is an input parameter of the routine called for the new smoothing occurrence, replacing the impulse function initially used. The new output response then takes into account both smoothing operations, ensuring that the final values of standardized vertical resolution are theoretically and numerically exact.

In the digital filter definition case, the plug-in routine not only outputs the vertical resolution, but also the gain of the filter over the entire spectrum of the frequency domain. When multiple smoothing operations occur within the same data processing chain, the plug-in routine is again called each time smoothing occurs, and the gain output by the routine during the previous smoothing occurrence is multiplied by the gain computed by the routine for the new smoothing occurrence. The product is a new gain that takes into account both smoothing operations, and from which the cut-off frequency is ultimately extracted. This way, the values of standardized vertical resolution output by the plug-in routine are once again conceptually, theoretically and numerically exact.

# 2 Standardized ozone and temperature uncertainty budget

The second objective of the ISSI Team was to recommend standardized definitions and approaches for the treatment of uncertainty in the NDACC lidar ozone and temperature lidar retrievals. Again, the recommendations were designed so that they can be implemented consistently by all NDACC ozone and temperature lidar investigators. The treatment of uncertainty in the ozone and temperature lidar retrievals depends on the choice of the theoretical equations used as well as their implementation to the real world, i.e., after considering all the caveats associated with the design, setup, and operation of an actual lidar instrument. There is therefore no unique answer or solution, but the ISSI Team made specific efforts to produce a set of actionable recommendations and suggest generic approaches that can be adapted to all cases.

## 2.1 Standardized definition of uncertainty

The definition of uncertainty recommended to be used for all NDACC lidar measurements is *combined standard uncertainty*. It originates in the two internationally recognized reference documents endorsed by the Bureau des Poids et Mesures (BIPM), namely the International Vocabulary of Basic and General Terms in Metrology (commonly abbreviated "VIM") (JCGM 200, 2012), and the Guide to the Expression of Uncertainty in Measurement (commonly abbreviated "GUM") (JCGM 100: 2008). These two documents and their supplements provide a complete framework to the treatment of uncertainty. The particular case of "standard uncertainty" is defined in the VIM as "*the measurement uncertainty expressed as a standard deviation*".

## 2.2 Standardized approach for the introduction and propagation of uncertainty

The same theoretical equation, namely the *lidar equation* (e.g., Hinkley, 1976), is used to retrieve an ozone number density profile in the troposphere or stratosphere using the DIAL technique (e.g., Mégie et al., 1977), and a temperature profile in the stratosphere and mesosphere using the density integration technique (e.g., Hauchecorne and Chanin, 1980). The parameters impacting the retrievals relate to the propagation and backscattering of the laser light emitted by the lidar, and therefore include a number of atmospheric species and their scattering and/or absorption properties. Furthermore the lidar equation relates to the number of photons collected on the lidar detectors rather than the raw lidar signals recorded in the data files. Therefore, several signal correction procedures and numerical transformations related to the instrumentation must be included as well. The effects of the data recorders, namely the sky and electronic background noise and the signal saturation (pile-up effect) must be taken into account.

One important recommendation by the ISSI team is to propagate all the individual, independent uncertainty components in parallel through the data processing chain. It is only after the final signal transformation is applied (i.e., leading to the actual values of ozone number density or temperature) that the individual uncertainty components are combined together to form the *combined standard uncertainty*, the primary and mandatory variable of the new NDACC-lidar-standardized ozone and temperature uncertainty budget. The expression of the individual uncertainty components and their step-by-step propagation through the ozone and temperature data processing chains was thoroughly estimated by the ISSI Team. The validity of the approach and correctness of the recommended expressions were quantitatively verified using simulated lidar signals and Monte Carlo experiments. The complete uncertainty propagation expressions and the validation experiments are detailed in the report.

### 2.2.1 Ozone DIAL retrieval

For the ozone DIAL retrieval, the independent sources of uncertainty identified by the ISSI Team are:

1) Random noise associated with signal detection
2) Uncertainty due to saturation correction (photon-counting mode only)
3) Uncertainty due to background noise extraction
4) Uncertainty due to channel merging procedure
5) Uncertainty due to the *a priori* use of ozone cross-sections
6) Uncertainty due to the *a priori* use of Rayleigh cross-sections
7) Uncertainty due to the *a priori* use of air number density (or temperature and pressure)
8) Uncertainty due to the *a priori* use of $NO_2$ absorption cross-sections
9) Uncertainty due to the *a priori* use of $NO_2$ number density (or mixing ratio)
10) Uncertainty due to the *a priori* use of $SO_2$ absorption cross-sections (UV only)
11) Uncertainty due to the *a priori* use of $SO_2$ number density (or mixing ratio)
12) Uncertainty due to the *a priori* use of $O_2$ absorption cross-sections (at shorter UV wavelengths)

The term *a priori* here does not mean that the ozone DIAL retrieval uses a variational/optimal estimation method (it does not), but simply means that the information comes from ancillary (i.e., non-lidar) measurements, and is input as "truth" in the data processing chain for use in the various lidar signal corrections needed. Not all of the above sources are necessarily needed, depending on the instrument configuration. All the above sources 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. In addition, if the same detection hardware is shared by two channels, the covariance terms must be taken into account when dependent channels are combined (e.g., signal merging or signal ratio). When computing the ozone cross-section differentials and the interfering gases' cross-section differentials, the covariance terms should also be taken into account if the same ancillary datasets are used for the "ON" and "OFF" wavelengths.

### 2.2.2 Temperature retrieval

For the temperature retrieval, the independent sources of uncertainty identified by the ISSI Team are:

1) Random noise associated with signal detection

2) Uncertainty due to saturation correction (photon-counting mode only)
3) Uncertainty due to background noise extraction
4) Uncertainty due to channel merging procedure
5) Uncertainty due to the *a priori* use of ozone cross-sections
6) Uncertainty due to the *a priori* use of ozone number density (or mixing ratio)
7) Uncertainty due to the *a priori* use of Rayleigh cross-sections
8) Uncertainty due to the *a priori* use of air number density (or temperature and pressure)
9) Uncertainty due to the *a priori* use of $NO_2$ absorption cross-sections
10) Uncertainty due to the *a priori* use of $NO_2$ number density (or mixing ratio)
11) Uncertainty due to the *a priori* use of temperature tie-on at the top of the profile
12) Uncertainty due to the *a priori* use of acceleration of gravity
13) Uncertainty due to the *a priori* use of molecular mass of air

Again the term *a priori* here simply means that the information comes from ancillary measurements, and is input as “truth” in the data processing chain for use in the signal corrections. Just like for ozone, not all of the above sources are necessarily needed, depending on the instrument configuration.

## 2.3 Reporting uncertainty in the NDACC data and meta-data files

As part of the ISSI team recommendations, every identified source of uncertainty should be reported in the NDACC-archived metadata file. Though not mandatory, providing quantitative information on the ancillary datasets used for signal corrections is highly recommended. The best estimate of the ozone (or temperature) combined standard uncertainty must be reported in the NDACC-archived lidar data files, whether or not the NDACC-standardized uncertainty budget approach recommended by the ISSI Team is used. The ISSI Team also recommends reporting, whenever possible, the individual standard uncertainty components that contribute to the reported ozone or temperature combined standard uncertainty.

Typical NDACC ozone and temperature lidar profiles are given as a function of altitude and for an averaging time period ranging between a few minutes and several hours. The ISSI Team recommends that information on individual uncertainty components should include the uncertainty source’s expected degree of correlation in both the altitude and time dimensions. The ISSI Team formulated basic recommendations on how to use the reported information when using a large set of profiles from the same lidar instrument (for example to produce an ozone or temperature climatology). Each reported individual uncertainty component must be first computed separately using the provided degree of correlation in altitude and time, and then combined. For example, uncertainty owed to detection noise should be computed using the quadratic sum of each individual profile’s detection uncertainty, while the uncertainty owed to the saturation correction can be combined using a simple sum of the individual profiles’ saturation correction uncertainty if the same correction procedure was used for all individual profiles.

## 3 Other aspects of the lidar ozone and temperature algorithms investigated

The ISSI Team reviewed several aspects of lidar data processing impacting the retrieved ozone and temperature profiles. The results detailed in the report include.

1) Recommendations on how to handle specific uncertainty sources and corrections

2) Recommendations on how to handle uncertainty associated with fundamental physical constants

3) A non-exhaustive list of ancillary datasets currently available (e.g., climatologies such as WACCM and GOZCARDS, satellite and balloon-borne measurements, and assimilation models) and their uncertainty

4) A comparison of the newest absorption cross-section datasets available (e.g., Univ. of Bremen spectroscopy data for ozone) with older datasets already in use by the atmospheric science community

5) A brief review of the Rayleigh cross-section formulas

6) Recommendations on how to handle uncertainty owed to co-location.

Uncertainty components due to particulate extinction and backscatter were not investigated by the ISSI Team. These terms are very small in a "clean" atmosphere, which is mostly true above 35 km and in most cases of tropospheric ozone DIAL measurements with a small wavelength differential. When present and non-negligible (for example after a large volcanic eruption), their contribution is highly variable from site to site, time to time, and highly dependent on the nature and quantity of the particulate matter at the time of measurement, which precludes the ISSI-Team from providing standardized expressions. However, the ISSI team is very aware that these terms certainly deserve full attention, and is urging for the formation of another Team of expert specifically dedicated to this topic. Finally, because every lidar instrument is unique, not all sources of uncertainty could be investigated by the ISSI-Team. For sources not treated in the ISSI team Report, the ISSI team recommends that the NDACC lidar investigators use the same generic approach as that proposed by the ISSI Team, and simply add those unidentified components to the uncertainty budget following the same definitions, methodologies, and propagation principles.

## 4 Validation of the proposed approaches, definitions and expressions

The values of vertical resolution following the proper standardized definitions were validated by the ISSI-Team using Monte-Carlo experiments for several NDACC ozone and temperature data processing softwares. The experiments consisted of 1) producing simulated lidar signals containing noise of frequencies covering the whole spectrum, 2) analyzing the simulated signals to retrieve temperature or ozone, and 3) comparing the retrieved profiles with the original profiles used to simulate the lidar signals. Besides validating the proper computation of standardized vertical resolution, these experiments show that the computed NDACC-standardized vertical resolution does not necessarily correspond to the width of the filtering window.

Because of the complexity of the ozone and temperature lidar uncertainty budgets, it is not possible to provide plug-in routines for uncertainty similar to those provided for vertical resolution. However, the approach, definitions, and propagation expressions are fully detailed in the report and can be used by the PIs as needed. Again, the approach and formulations were quantitatively verified using Monte-Carlo experiments involving simulated lidar signals. In this case the purpose of the experiments was to propagate normally distributed perturbations of the input parameters contributing to the ozone or temperature uncertainty budget, and verify that the data processing algorithms compute values of ozone or temperature standard uncertainty that are equal to the ozone or temperature standard deviation obtained from the set of perturbed signals. The results of these experiments are fully detailed in the report.

# 5 Extension of the ISSI Team work to the water vapor and aerosol lidars

The recommendations and approaches proposed by the ISSI Team for the NDACC ozone and temperature lidars can be largely extended to the NDACC water vapor and aerosol lidars. In particular, the recommendations and approaches pertaining to the lidar signal processing common to both ozone and temperature (i.e., background extraction, saturation correction, smoothing and merging at the signal level or at the species level, and the standardization of vertical resolution), can easily be implemented in a similar manner for the backscatter ratio and water vapor profiles. Uncertainty components that are specific to the retrieval of aerosol properties or water vapor profiles (e.g., calibration) can be further investigated following a philosophy and approach that are similar to those described in the ISSI Team Report.

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