GAIA-CLIM Report

Gap Analysis for Integrated Atmospheric ECV CLImate Monitoring:

Final review of and update to the GAID from the perspective of WP2

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Table of Contents

Introduction

The GAIA-CLIM project aims to assess and improve global capabilities to use ground-based, balloon-borne, and aircraft measurements (termed non-satellite measurements henceforth) to characterise space-borne satellite measurement systems. The work under GAIA-CLIM encompasses the following tasks:

1. Defining and mapping existing non-satellite measurement capabilities;
2. Improving the metrological characterisation of a subset of non-satellite (reference) observational techniques;
3. Better accounting for co-location mismatches between satellite observations and non-satellite (reference) observations;
4. Exploring the role of data assimilation as an integrator of information;
5. Creation of a 'Virtual Observatory' bringing together all comparison data, including their uncertainties, and providing public access to the information they contain;
6. Identifying and prioritizing gaps in knowledge and capabilities. Under its work package 6, GAIA-CLIM performs an assessment of gaps in capabilities or knowledge relevant to the use of non-satellite data to characterise satellite measurements.

It is recognized that GAIA-CLIM shall provide progress in these application areas, but not necessarily close out all potential issues and challenges. Hence, in each of the project tasks outlined above, presently unfulfilled user needs ('gaps') have been identified through an iterative process throughout the project's lifetime. This gaps assessment exercise exclusively considers gaps identified as relevant to these GAIA-CLIM project aims. The identified key user communities for whom the impact of the identified gaps would be most relevant include:

- Service providers (e.g. ECMWF for NWP, CAMS and C3S)
- Users and providers of ECV climate data records (e.g. space agencies and satellite data user communities)
- Users of reference observations
- Users of baseline network observations
- Users of the 'Virtual Observatory'

The Gaps Assessment and Impacts Document (GAID) is a living document that summarises the outcome of this collection of gaps and their proposed remedies. It further describes the gap identification process, as well as the way these findings are presented and made accessible to users, stakeholders and actors. The current set of gaps and remedies captured under the living GAID document v4 provides a firm basis for providing costed and prioritised recommendations for future work to improve our ability to use non-satellite data to characterise satellite measurements. The first draft of the recommendations document[1] builds upon this careful and meticulous collection and cataloguing process to produce a set of eleven overarching recommendations for future work to close the most critical gaps identified through the life of the project.

This document provides a snapshot of the gaps status as per December 2017 in relation to work package 2. It provides a third, and final, formal delivery of WP2 input to the process. The on-line 'Catalogue of Gaps' provides the latest version of the full content of the gaps and their proposed remedies. The catalogue is available from: http://www.gaia-clim.eu/page/gap-reference-list.

[1] http://www.gaia-clim.eu/page/recommendations

Input from external parties continues to be invited through the GAID website. A designated e-mail address[2] and a specific template for gap reporting is provided at the website. Further user engagement shall be achieved through a series of visits to key stakeholders through the end of 2017. This user feedback will be important in refining the GAID and ensuring its usefulness to the broader scientific and policymaker communities, as well as space agencies, international organisations, and funding bodies.

[2] Email address for GAID feedback: gaid@gaia-clim.eu

1. Summary of existing gaps for WP2

Table 1.1. Overview of the gaps identified under work package 2 under GAID V4 and their identified remedies. The table entries reflect modified titles and changes to remedies proposed in the current deliverable. Note that G2.34 has been resolved and hence removed as outlined in Section 2.

Gap reference	Gap title	Remedies
G2.06	Current poor spatial coverage of high-quality multi-wavelength lidar systems capable of characterising aerosols	• (R1) Improve the coverage, metrological characterisation, and operational capabilities of Raman lidars
G2.07	Lack of uptake of lidar measurements in data assimilation	• (R1) Extension of the GAIA-CLIM data-assimilation approach to aerosol lidars
G2.08	Need for a metrologically rigorous approach to long -term water vapour measurements from Raman lidars in the troposphere and UT/LS	• (R1) Synergy between water vapour Raman lidar and other measurement techniques • (R2) Verification and further deployment of the GAIA-CLIM approach to metrological characterisation to Raman Lidar measurements
G2.10	Tropospheric ozone profile data from non-satellite measurement sources is limited and improved capability is needed to characterise new satellite missions	• (R1) Expand coverage of differential absorption lidars to improve ability to characterise tropospheric ozone
G2.11	Lack of rigorous tropospheric ozone lidar error budget availability	• (R1) Create and disseminate a fully traceable reference-quality DIAL lidar product
G2.12	Lack of rigorous pure rotational Raman temperature lidar error budget availability limits utility for applications, such as satellite characterisation	• (R1) Create a fully traceable reference-quality temperature lidar product
G2.13	Missing microwave standards maintained by national/international measurement institutes	• (R1) Development and testing of MWR standards and secondary standards
G2.18	Better agreement needed on systematic and random components of the uncertainty in FTIR measurements and how to evaluate them	• (R1) Improved traceability of uncertainties in FTIR measurements
G2.22	FTIR cell measurements carried out to characterize Instrument Line Shape have their own uncertainties	• (R1) Regular cell measurements and ILS retrievals are to be performed in a consistent manner
G2.24	Lack of calibrated in-situ vertical profiles of CH_4, CO_2 (and CO) for improving the accuracy of FTIR (partial) column measurements of CH_4, CO_2 (and CO)	• (R1) Operationalise the Aircore technique at a range of sites also measuring using FTIR • (R2) Enhance the airborne infrastructure in Europe • (R3) Create a database of in-situ vertical profiles of CO_2, CH_4, and CO with sufficient spatiotemporal coverage, possibly as part of the ICOS RI
G2.26	Poorly understood uncertainty in ozone cross-sections used in the spectral fit for DOAS, MAX-DOAS, and Pandora data analysis	• (R1) Improved understanding of the effects of differences in ozone cross-sections

G2.27	Lack of understanding of random uncertainties, air mass factor calculations, and vertical averaging kernels in the total ozone column retrieved by UV-visible spectroscopy	• (R1) Improve our understanding of the discrepancy between the calculated fitting uncertainty and the more realistically estimated total random error • (R2) Improvements to climatological databases of a priori ozone profiles for use in retrievals • (R3) Standardize AMF calculation methods and databases of a-priori information used in AMF calculations to improve accuracy of the measured total column ozone • (R4) Evaluation of 3D averaging kernels for zenith-sky UV-visible ozone measurements
G2.30	Metrologically incomplete uncertainty quantification for Pandora ozone measurements	• (R1) Steps towards reference quality measurement program for Pandora measurements
G2.31	Incomplete metrological understanding of the different retrieval methods, information content, and random and systematic uncertainties of MAX-DOAS tropospheric ozone measurements	• (R1) Improved metrological understanding of potential for MAX-DOAS high-quality measurements and retrieval techniques of tropospheric ozone.
G2.36	Lack of traceable uncertainties in MWR measurements and retrievals	• (R1) Adoption of an international approach to implement recommendations for addressing existing gaps in MWR operational products for climate-monitoring utilization
G2.37	Need for more complete metrological characterisation of spectroscopic information	• (R1) Establish traceability of spectroscopic properties of Essential Climate Variables

2. Detailed update on traces for the gaps arising from WP2

The changes made to the existing gaps identified as relevant for the WP2 activities are based on the following motivations:

- The need for an updated description of gaps and remedies linked to the timing and the progress of the activities carried out within GAIA-CLIM and other EU or international projects;
- The project progress which has contributed to the refinement of the gap analysis since the last version of the GAID;
- Improved knowledge of the motivation behind the gaps and an enhanced capability to clarify the description of gaps and remedies.

Specific important content edits, beyond grammatical tidying and small clarifications, which have been applied in all cases per gap are as follows:

G2.06: "Current poor spatial coverage of high-quality multi-wavelength lidar systems capable of characterising aerosols"

Updates to the title and text of the remedy have been applied. Some aspects of G2.06 have been resolved within the GAIA-CLIM project, but overall, the gap will remain. The remedy has been rewritten in such a manner that it provides a better-defined unit of potential work and the title of the remedy has been changed as well to reflect this.

G2.07: "Lack of uptake of lidar measurements in data assimilation"

The remedy has been updated so it is more focussed on the precise remit of the work being suggested and to this end, a more specific work plan has been included. As previously envisaged, G2.07 will remain unresolved.

G2.08: "Need for a metrologically rigorous approach to long-term water vapour measurements from Raman lidars in the troposphere and UT/LS"

One remedy entitled "Synergy between water vapour Raman lidar and other measurement techniques" has been added and the second remedy has been changed to reflect some clarifications. G2.08 has been partially addressed within WP2 but will overall stay unresolved.

G2.10: "Tropospheric ozone profile data from non-satellite measurement sources is limited and improved capability is needed to characterise new satellite missions"

Only a small addition to the remedy description has been made. G2.10 has not been addressed within GAIA-CLIM.

G2.11: "Lack of rigorous tropospheric ozone lidar error budget availability"

Some additional text to the gap description and remedy has been given, and work pursued within GAIA-CLIM is leading to a partial resolution of the gap by further developing a rigorous uncertainty budget for tropospheric ozone profiles using the DIAL lidar technique. However, some work remains to be undertaken to deploy the developed technique.

G2.12: "Lack of rigorous pure rotational Raman temperature lidar error budget availability limits utility for applications, such as satellite characterization"

The title for G2.12 has been changed to emphasize that the temperature measurements discussed under this gap are measured using the pure-rotational Raman (PRR) technique and this has been followed through in other parts of the text as well. This gap has not been addressed within GAIA-CLIM.

G2.13: "Missing microwave standards maintained by national/international measurement institutes"

Minor updates to the contents and title, and in particular to the references, have been applied and this gap has been partly closed by GAIA-CLIM. As envisaged right from the beginning, G2.13 cannot be resolved within GAIA-CLIM but needs to be addressed by the relevant national/international measurement institutes and communities with GAIA-CLIM's task having been to highlight the gaps, review the developments and progress, and to report back to the community.

G2.18: "Better agreement needed on systematic and random components of the uncertainty in FTIR measurements and how to evaluate them"

Some content, especially in the detailed gap description, has been added and a small change has been applied to the title. Although GAIA-CLIM contributed to closing the gap by promoting recipes to evaluate random and systematic parts of the uncertainty sources, that does not mean yet that they will be implemented at each FTIR site by the end of GAIA-CLIM and the gap will thus remain open.

G2.22: "FTIR cell measurements carried out to characterize Instrument Line Shape have their own uncertainties"

Some content has been added, especially within the proposed remedy, and a small change has been applied to the title. Although progress has been made within GAIA-CLIM to identify the contribution of the Instrument Line Shape (ILS) uncertainty to the total uncertainty budget and to make it better traceable, the harmonization between the different retrieval software packages is not complete yet, and the implementation within all FTIR stations needs to still be done consistently. Hence, this gap will remain open.

G2.24: "Lack of calibrated in-situ vertical profiles of CH_4, CO_2 (and CO) for improving the accuracy of FTIR (partial) column measurements of CH_4, CO_2 (and CO)"

The contents of the gap description have been quite substantially changed. The previously identified risk entry has been replaced with three new ones and the previously discussed remedy has also been replaced by three new ones. Furthermore, the title has been updated as well. This gap will remain unresolved.

G2.26: "Poorly understood uncertainty in ozone cross-sections used in the spectral fit for DOAS, MAX-DOAS, and Pandora data analysis"

Some content has been added, in particular to the proposed remedy. The gap topic has been reviewed within GAIA-CLIM, but the gap will remain after the GAIA-CLIM project has been completed.

G2.27: "Lack of understanding of random uncertainties, air mass factor calculations, and vertical averaging kernels in the total ozone column retrieved by UV-visible spectroscopy"

Some clarifying text has been added. In particular all four remedies have been further developed and clarified. Some component of G2.27 has been addressed within GAIA-CLIM, e.g. the in-depth uncertainty analysis of total column ozone. However, the gap itself will remain.

G2.30: "Metrologically incomplete uncertainty quantification for Pandora ozone measurements"

More details have been added to the proposed remedy and the title had a small addition. G2.30 has been partially addressed within GAIA-CLIM, but needs to be addressed further in collaboration with the Pandora community and in context of the findings soon to be available based on the CINDI-2 campaign, held in September 2016, i.e. the gap remains.

G2.31: "Incomplete metrological understanding of the different retrieval methods, information content, and random and systematic uncertainties of MAX-DOAS tropospheric ozone measurements

The two remedies previously proposed for this gap have been merged into one. This gap has been partly addressed during the time frame of GAIA-CLIM, in particular through the work done by the CINDI-2 MAX-DOAS Tropospheric Ozone Working Group, but many aspects of the gap remain.

G2.34: "Limit in traceability of GNSS-IPW ZTD estimates owing to dependency on 3rd party software"

This gap was closed because GAIA-CLIM activities under work package 2 confirmed that the main issue leading to significantly different ZTD uncertainty values (via an example of GAMIT and Bernese approaches) comes from different initial constraints for uncertainty analysis in the software. These findings and their implications will be further outlined in the Task 2.1 Deliverable D2.8.

G2.36: "Lack of traceable uncertainties in MWR measurements and retrievals"

The changes to G2.36 have been minor apart from a clarification of the title of the proposed remedy and the addition of several references. This overarching MWR gap will remain for now but will be considered closed once procedures for MWR calibration and instrument characterization, and a unified retrieval method have been applied uniformly across the network.

G2.37: "Need for more complete metrological characterisation of spectroscopic information"

Some modifications have been made to the contents of this gap, with additional detail added to the remedies, and the title has been adjusted. This top-level gap regarding uncertainty quantification in spectroscopic information will remain after the GAIA-CLIM project has finished.

3. Conclusions

This deliverable and the gap traces contained in Annex I constitute the third and final official input to the GAID process arising from WP2. The WP2 input to the GAID has evolved substantively throughout the project. It is clear that further advances could be achieved were investment and expertise available to undertake the steps described herein to improve the metrological quantification for a broad range of ground-based and in-situ measurement technologies.

4. Annex I Updated GAIA-CLIM Catalogue of gaps for WP2

Within this section gaps that were detailed in section 1 are here expanded to give full trace of the current understanding of the gaps including a revision of its impacts and potential remedies.

G2.06 Current poor spatial coverage of high-quality multi-wavelength lidar systems capable of characterising aerosols

Gap abstract:

Raman lidars or multi-wavelength Raman lidars are undoubtedly an integral component of an aerosol global measurement infrastructure as they can provide quantitative range-resolved aerosol optical and microphysical properties. It is very important to carefully assess the value of the retrieval of advanced lidar systems and to study if the global coverage of the existing networks is sufficient to carry out adequate satellite-retrieval characterisation. The availability of a larger number of multi-wavelength Raman lidar measurements would strengthen the global observing system for the upcoming research satellite mission Cal/Val (Sentinels 4/5, ADM-Aeolous, Earth-CARE, ACE) and ensure a critical contribution to distinguish natural and anthropogenic aerosols from satellite data. Multi-wavelength Raman lidars could be considered to be the future backbone of a larger network incorporating simpler lidar instruments and/or ceilometers, and so be able to have a denser global spatial coverage.

Part I: Gap description

Primary gap type:

Spatiotemporal coverage

ECVs impacted:

Aerosols

User category/Application area impacted:

- Operational services and service development (meteorological services, environmental services, Copernicus Climate Change Service (C3S) and Atmospheric Monitoring Service (CAMS), operational data assimilation development, etc.)
- Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)

Non-satellite instrument techniques involved:

Lidar

Detailed description:

Raman lidars or multi-wavelength Raman lidars are undoubtedly an integral component of an aerosol global measurement infrastructure as they can provide quantitative range-resolved aerosol optical and microphysical

properties throughout much of the column. Whereas the detection of aerosol layers and their vertical extent requires only simple single wavelength backscatter lidars, the derivation of extinction coefficient profiles and of a series of derived aerosol properties requires advanced lidar setups and techniques such as high-spectral resolution lidars (Shipley et al., 1983) or Raman lidars (Ansmann et al., 1992). The estimation of aerosol microphysical properties and mass concentration requires at a minimum a one-wavelength Raman lidar, though the error affecting these estimations can be dramatically reduced if a multi-wavelength Raman lidar system is used. This highlights the relevance of having an enhanced number of multi-wavelength Raman lidars globally if they are to be used to characterise satellite measurements that aim to discern such properties.

Such lidars also have a potential role as anchor reference stations for the study of the impact of aerosols on weather and climate more generally. The availability of multi-wavelength Raman lidar measurements also ensures that ground-based instruments can deliver wavelength conversion information for different aerosol and cloud types to relate the current and future space-borne measurements performed by different satellite missions at different wavelengths (for example, CALIPSO at 532 nm and the future EarthCARE mission at 355 nm). In addition, space-based measurements have the advantage of obtaining global spatial coverage, but long-term ground-based observations can provide a critical contribution to distinguish natural and anthropogenic aerosols from satellite data.

Multi-wavelength Raman lidars could be considered to be the future backbone of a larger network incorporating simpler lidar instruments and/or ceilometers, and so be able to have a denser global spatial coverage. In this process, it is very important to carefully assess the value of the retrieval of advanced lidar systems and to study if the coverage of the existing networks globally is sufficient to carry out a sufficiently accurate aerosol study.

Steps towards automatic or semi-automatic usage of the most advanced lidars are needed to reduce the traditional intensive manpower typically required to operate these systems. In this sense, the effort spent over the last year by the biggest aerosol lidar networks (EARLINET, MPLnet) to develop an automatic lidar data processing chain must be acknowledged.

The working groups of lidar network representatives involved in the Aerosol SAG (Scientific Advisory Group) of the WMO-GAW programme has recently started working to address (on voluntarily basis) specific harmonisation issues on a global scale.

Operational space missions or space instruments impacted:

- Copernicus Sentinel 4/5
- Active sensors

Validation aspects addressed:

Time series and trends

Gap status after GAIA-CLIM:

After GAIA-CLIM, this gap remains unaddressed.

Some activities pertinent to this gap have been addressed but the gap could not be solved completely within the timeframe of GAIA-CLIM.

Part II: Benefits to resolution and risks to non-resolution

Identified benefit	**User category/Application area benefitted**	**Probability of benefit being realised**	**Impacts**
Improved coverage of aerosol lidar measurements at a global scale	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Increase the accuracy of estimation of aerosol effects on weather and climate; improved monitoring of aerosol related natural hazards e.g. volcanic plumes, dust storms
Stronger global observing system for the upcoming research satellite Cal/Val (e.g. for missions like ADM-Aeolus, EarthCARE, Sentinels).	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High Medium	Availability of Fiducial Reference Measurements (FRM) for ensuring the harmonization of satellite data products
Identified risk	**User category/Application area benefitted**	**Probability of benefit being realised**	**Impacts**
Lower spatial coverage for satellite validation using Raman lidar measurements	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	Medium	There is a continuously increasing demand for aerosol products for different applications (climate, weather, satellite, air quality, solar applications, agriculture, health), but quantitative measurements of aerosol microphysical properties in the column can only be provided by Raman lidar systems, the good spatial coverage of which is also essential for the calibration of baseline observations (i.e. ceilometers).
		High	

Need for the harmonization of aerosol satellite measurements performed at different wavelengths	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)		Over coming decades, the number of aerosol satellite missions will increase and this requires the establishment of databases containing the conversion factors to allow a physically consistent use of measurements performed at different wavelengths, as described in Pappalardo et al., 2010 (JGR). The risk is to have non-harmonized CDRs that cannot effectively contribute to the interpretations of global climate change.

Part III: Gap remedies

Gap remedies:

Remedy 1: Improve the coverage, metrological characterisation, and operational capabilities of Raman lidars

Primary gap remedy type:

Deployment

Proposed remedy description:

A first step would be to identify existing Raman lidar measuring aerosol properties globally and then subsequently study the representativeness of each station in the characterization of aerosol variability in a range of different vertical atmospheric regions. This would allow the identification of those priority climatic regions where additional multi-wavelength Raman lidars are required and taking advantage of existing lidar stations which are not operating a Raman lidar yet.

To make such activities sustainable and operational at a global scale, many further steps are needed, including:

a. Establishment of mechanisms for regular communication between networks (under GAW coordination);
b. Developing an agreement on a shared/common metadata access portal and automatic product calculation;
c. Improving the metrological characterisation of many systems (e.g. existing assessments indicate some potential systematic errors in the aerosol characterisation);
d. Developing common harmonised methodologies, data quality objectives, quality assurance/quality control procedures across measurement frameworks to the extent possible;
e. Performing frequent intercomparison activities.

Relevance:

A complete remedy for this gap is strongly related to the strategies of the international research institutions which are at present the key players in the deployment and the operation of Raman lidar measurements. A well-defined strategy implementing integration of aerosol measurement capabilities on continental or larger scales will result in clear benefits such as improved data access and availability, improved comparability of data, more uniform data quality standards from different networks, increased synergy of measurements and prevention of unnecessary duplication.

Commercial lidars or ceilometers will benefit of an improved metrological characterization, with a consequent impact of the ingestion of massive higher quality data from low-cost monitoring systems in real-time within weather numerical models.

Measurable outcome of success:

This is obviously related to the establishment of multi-wavelength Raman lidars in those regions where a lack of lidar instruments is identified by a study of representativeness of the existing measurements of aerosol properties. Such study also allows a rationalization of the required investments.

Expected viability for the outcome of success:

Medium

Scale of work:

- Single institution
- Consortium

Time bound to remedy:

Less than 5 years

Indicative cost estimate (investment):

Medium cost (< 5 million)

Indicative cost estimate (exploitation):

Yes

Potential actors:

- National funding agencies
- ESA, EUMETSAT or other Space agency
- Academia, individual research institutes

References:

- Ansmann, A., U. Wandinger, M. Riebesell, C. Weitkamp and W. Michaelis, Independent measurement of extinction and backscatter profiles in cirrus clouds by using a combined Raman elastic-backscatter lidar. Applied optics, 31, 7113, 10.1364/AO.31.007113, 1992.

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- World Meteorological Organisation, Global Atmosphere Watch, Recommendations for a Composite Surface-Based Aerosol Network. GAW Report No. 207, http://www.wmo-gaw-wcc-aerosol-physics.org/files/gaw-207.pdf.

G2.07 Lack of uptake of lidar measurements in data assimilation

Gap abstract:

Aerosol lidar data can potentially be used to constrain uncertain model processes in global aerosol-climate models. Satellite-borne lidar data can be effectively assimilated to improve model skill but, currently, aerosol lidar data assimilation experiments are mainly limited to the assimilation of attenuated backscatter, which is a non-quantitative optical property of aerosol. There is much additional valuable data that could be utilised to improve data assimilation. Such improved data assimilation may allow attenuation of data to allow broader inferences about satellite quality as being developed by GAIA-CLIM for temperature and humidity via the GRUAN processor.

Part I: Gap description

Primary gap type:

Knowledge of uncertainty budget and calibration

ECVs impacted:

Aerosols

User category/Application area impacted:

- Operational services and service development (meteorological services, environmental services, Copernicus Climate Change Service (C3S) and Atmospheric Monitoring Service (CAMS), operational data assimilation development, etc.)
- International (collaborative) frameworks and bodies (SDGs, space agencies, EU institutions, WMO programmes/frameworks etc.)

Non-satellite instrument techniques involved:

Lidar

Detailed description:

Uncertainties associated with aerosol emissions in terms of their intensity and distribution pattern, atmospheric processes, and optical properties, represent a significant part of the uncertainty associated with the quantification of the impact of aerosols on climate and air quality in regional and global models. Lidar assimilation in global aerosol-climate models is an active area of research at many forecasting centres and research institutes. Assimilation systems used range from variational to ensemble methods, variables assimilated are aerosol extinction and backscatter coefficients or lidar raw signals (by using customized forward models). Applications range from aerosol global forecasts, to volcanic ash detection and regional air quality.

Data assimilation techniques are implemented to decrease these uncertainties, constraining models with available information from observations in order to make a best estimate of the state of the atmosphere. The short-range forecasts from such systems have the potential to be useful for the calibration/validation (Cal/Val) of new satellite data as they provide a stable reference for inter-comparison between products from different satellites. In particular, the use of a forecast model minimises errors due to temporal differences when comparing two different observational datasets.

This Cal/Val technique has been found to be useful for satellite observations sensitive to temperature and humidity, since the short-range forecasts are highly accurate for these variables, and this has been explored further within the GAIA-CLIM project. However, for aerosol products the short-range forecasts are not yet accurate enough to be able to identify more than gross errors in the satellite observations.

Further improvements to the aerosol data assimilation systems are needed, particularly in the area of bias correction, before aerosol forecasts can be used as a reference for satellite Cal/Val. This is a long-term goal, however, and in the short-term direct comparisons between aerosol observations should continue to be carried out for the Cal/Val of new satellite products.

Aerosol lidar data can also be used to constrain uncertain model processes in global aerosol-climate models. Satellite-borne lidar data can be effectively assimilated to improve model skill but, currently, aerosol lidar data assimilation experiments are mainly involving lidar attenuated backscatter, which is a non-quantitative optical property of aerosol. Ground based lidar networks can in addition provide quantitative measurements of aerosol backscatter and extinction coefficients. However, a limited number of aerosol lidar data assimilation experiments have been performed, preventing us from assessing the effective impact of assimilating continuous satellite lidar data and whether the current state of the lidar technology fulfils the modellers' needs.

Operational space missions or space instruments impacted:

- Copernicus Sentinel 4/5
- Active sensors

Validation aspects addressed:

- Assimilated product (Level 4)

Gap status after GAIA-CLIM:

After GAIA-CLIM, this gap remains unaddressed.

GAIA-CLIM has undertaken no specific activities to help addressing this gap.

Part II: Benefits to resolution and risks to non-resolution

Identified benefit	User category/Application area benefitted	Probability of benefit being realised	Impacts

Improved model performances to determine aerosol effect at a global scale on weather and climate	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Reduction of the IPCC identified uncertainties related to the aerosol direct and indirect effects, with a consequent improvement of climate and weather forecast.
Identified risk	**User category/Application area benefitted**	**Probability of benefit being realised**	**Impacts**
Bias correction for satellite lidar data using a variational bias correction scheme not feasible	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) International (collaboration) frameworks (SDGs, space agency, EU institutions, WMO programmes/frameworks etc.)	High	Assimilation of satellite lidar data will continue to bias the model output instead of improving the forecast skills.
Larger uncertainty if aerosol lidar data are not used to constrain uncertain model processes in global aerosol-climate models.	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.)	High	Uncertainties associated with aerosol emissions impacts on climate and air quality simulations in regional and global models.

Part III: Gap Remedies

Gap remedies:

Remedy 1: Extension of the GAIA-CLIM data assimilation approach to aerosol lidars

Primary gap remedy type:

Research

Proposed remedy description:

New solutions for assessing and enhancing the value of lidar data assimilation must be developed. This requires efforts in two complementary areas:

1. Aerosol lidar networks must strongly work on their capability to provide NRT data, through the implementation of automatic processing calculus chains and to adopt shared/common metadata international standards in order to facilitate the data usage and manipulation.
2. Modellers must develop methodologies to use the available lidar Near-Real time (NRT) data for routine evaluation of operational models or data assimilation, through the development of improved forward operators, while quality-checked (QC) and added-value (higher level data) products must be used for the retrospective assessments of model simulations (reanalysis/reforecast).

Building on the growing interest from the global NWP community in using high accuracy data from ground-based networks to constrain satellite data biases, ground-based lidar data could be used by modellers also to anchor the bias correction for satellite lidar data, using a variational bias correction scheme.

However, further work must be implemented aimed at improving model skill, i.e models are better at predicting horizontal transport than vertical distributions. Formulation of a specified work plan should take into account that:

- Collaboration with data providers is paramount;
- NRT data delivery from all lidar satellite missions is important;
- With respect to other lidar measurements of atmospheric composition, the community is largely ready to use lidar data to improve aerosol predictions;
- Wind data will also improve atmospheric composition prediction by improving the model wind fields.

Relevance:

Aerosol is one the key factors in the determination of the radiative balance with its direct and indirect effect. An appropriate and successful assimilation within numerical models may strongly improve our climate knowledge as well as the prediction of severe weather events. This value is enhanced by the multitude of data which will be available at global scale – with the advent of upcoming satellite missions with a lidar technique on-board including the ESA missions, ADM-Aeolus and EarthCARE.

Measurable outcome of success:

A number of initiatives are currently ongoing and their outcome will give us within a few years a quantitative idea of the importance of using lidar measurements in data assimilation.

Expected viability for the outcome of success:

High

Scale of work:

Consortium

Time bound to remedy:

Less than 5 years

Indicative cost estimate (investment):

High cost (> 5 million)

Indicative cost estimate (exploitation):

Yes

Potential Actors:

- National Meteorological Services
- Academia, individual research institutes

G2.08 Need for a metrologically rigorous approach to long - term water vapour measurements from Raman lidars in the troposphere and UT/LS

Feedback

Gap abstract:

One of the paramount needs for developing long-term ECV datasets for atmospheric monitoring is to calibrate measurements using SI traceable standards. For water vapour measured with the Raman lidar technique, a solution is represented by the calibration of water vapour profiles using reference calibration lamps, which are traceable to NMIs standards. Another critical issue to ensure continuous water vapour Raman lidar measurement is due to the weakness of the Raman backscattering from water vapour molecules. During daytime, a few water vapour Raman lidars have already proven to be able to measure water vapour up to 3-4 km above ground level, but despite this, only a few of them are operated on a continuous basis. Technological improvements or the effective integration with other techniques needs to be pursued.

Part I: Gap description

Primary gap type:

Knowledge of uncertainty budget and calibration

Secondary gap type:

- Spatiotemporal coverage
- Vertical domain and/or vertical resolution

ECVs impacted:

Water vapour

User category/Application area impacted:

Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)

Non-satellite instrument techniques involved:

Lidar

Detailed description:

A long-term data set for monitoring atmospheric water vapour using lidar techniques requires the calibration of Raman lidar water vapour profiles that vary randomly around some mean value (often addressed as a calibration constant that depends only on the instrument setup) and does not involve step jumps of unknown magnitude. Such step jumps in calibration increase the time required to detect atmospheric trends, which is already typically measured in decades [Weatherhead et. al., 1998; Boers and Meijgaard, 2009]. For this reason, it is important to carefully examine any calibration technique developed for ensuring stable and long-term calibrations. Absolute and relative, but also hybrid calibration methods have been developed. More recently, reference calibration lamps, which are traceable to NMIs standards, have proven to be robust for absolute calibration of water vapour Raman lidar to reduce systematic uncertainties and may represent a common reference for all the available systems.

Another challenge for Raman lidars to ensure the collection of water vapour long-term measurements for climate applications is to improve their daytime observing capability. Raman lidars have been shown to provide high resolution water vapour measurements in several experiments, but these measurements are typically restricted to night-time only, as Raman scattering is a weak physical process and the high solar background radiation during the day tends to mask these signals. During daytime, a few water vapour Raman lidars have already proven to be able to measure water vapour up to 3-4 km above ground level. Only DIAL systems can do better, but they do worse in the UT/LS at night compared to Raman lidar. Most of the water vapour Raman lidar systems are not operated during daytime and this generates a discontinuity in the water vapour monitoring in the troposphere in a climatological sense. The use of commercial systems, Raman lidar or DIAL, designed to operate on a continuous basis, can mitigate the gap but with moderate to high costs, though their performance needs to be carefully assessed in advance. Further technological improvements of lidar techniques for measuring water vapour are also expected but over the mid and long term.

In addition, the improvement of synergy of water vapour Raman lidar with other measurement techniques represents an alternative solution upon which to invest. For example, the ACTRIS-2 and HD(CP) projects are working on this aspect to provide users with a synergetic lidar-radiometer water vapour product in both clear and cloudy sky conditions to cover the tropospheric range.

Operational space missions or space instruments impacted:

- MetOp-SG
- Microwave nadir
- Infrared nadir
- Passive sensors
- GNSS-RO

Validation aspects addressed:

Geophysical product (Level 2 product)

Gap Status after GAIA-CLIM:

GAIA-CLIM has partly closed this gap.

GAIA-CLIM has contributed to addressing this gap under activities associated with the metrological characterisation of instrumentation.

Part II: Benefits to resolution and risks to non-resolution

Identified benefit	**User category/Application area benefitted**	**Probability of benefit being realised**	**Impacts**
Harmonization of water vapour measurements and reduction of biases in the satellite validation	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Improved capability to detect signals of climate change
Continuous monitoring of water vapor in the troposphere and in the UT/LS in support of satellite validation and assimilation models	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Improved weather and climate forecasts
Identified risk	**User category/Application area benefitted**	**Probability of benefit being realised**	**Impacts**
Lack of harmonization between water vapor Raman lidars globally.	Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Inhomogeneities affecting water CDR in the troposphere and stratosphere to detect a signal of climate change.
Bias and lower performances in the intercomparison or in the retrieval of atmospheric state estimates from sensors synergy.	Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	Medium	Biased, lower vertical and temporal resolution of atmospheric best estimate profile; partially compensated by potential sensor intercalibration.
Measurement and temporal biases affecting datasets used for satellite validation.	Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	Medium	Limited quality and temporal resolution of lidar water vapour reference measurements available data for OSSE and satellite validation.

Part III: Gap remedies

Gap remedies:

Remedy 1: Synergy between water vapour Raman lidar and other measurement techniques.

Primary gap remedy type:

Laboratory

Proposed remedy description:

The synergy of water vapour Raman lidar with other measurement techniques, like GPS/GNSS, optical and microwave radiometry, etc., provides complementary information on the water vapour structure to constrain, extend or simply improve the quality of the information provided by lidar. In particular, synergy with passive microwave radiometers provides an robust solution to obtaining a low resolution profile of atmospheric water vapour during daytime also above the atmospheric altitude covered by lidar enabling the characterization of the entire atmospheric column: This could partially address this gap but this synergetic solution requires the development of new and more accurate algorithms to fully exploit the potential of the combined datasets. It also requires the co-location of these synergistic measurement techniques in close enough geographical proximity to be usable in this manner.

Relevance:

Continuous measurements of water vapour observations with high spatial (vertical) and temporal resolution are needed to achieve a comprehensive understanding of the role of water vapour on climate at regional and global scales as well as to estimate its impact on OLR = outgoing long- wave radiation (OLR) at top of atmosphere. The availability of water vapour profiles in both cloud and clear sky conditions would largely enhance several activities related to the study of climate, to satellite retrievals, and radiative transfer modelling. Furthermore, the synergetic approach to improve water vapour measurement continuity is at present the only chance to improve daytime water vapour profiling capabilities.

Measurable outcome of success:

Success of any kind of synergetic products or joint retrieval performed using Raman lidar and microwave radiometry (or other measurement techniques) shall be assessed by using the data in the input data stream of the mesoscale models or by validating the water vapour model output profiles. Alternatively, a comparison with radiosounding profiles from Reference networks (i.e. GRUAN) can represent another good way to assess the added values of this higher-level products though in this case the difference in the representativeness of the two different products (lidar+other vs radiosonde) must be quantified and taken in account.

Expected viability for the outcome of success:

- Medium
- High

Scale of work:

- Individually
- Single institution

Time bound to remedy:

- Less than 5 years

Indicative cost estimate (investment):

- Low cost (< 1 million)

Indicative cost estimate (exploitation):

Non-applicable

Potential actors:

- Academia, individual research institutes
- SMEs/industry
- National measurement institutes

Remedy 2: Verification and further deployment of the GAIA-CLIM approach to metrological characterisation to Raman Lidar measurements

Primary gap remedy type:

Laboratory

Proposed remedy description:

Work within GAIA-CLIM has advanced the metrological characterisation of raman lidar water vapour products. Verification of the results generated in GAIA-CLIM is required prior to broad-scale adoption of the traceable

measurement and processing approach by networks. At the same time work is required to improve the temporal coverage of measurements to increase their utility with a particular focus on advancing daytime measurements.

Relevance:

For water vapour lidar calibration, the proposed remedy will dramatically improve the traceability of water vapour Raman lidar measurements and data consistency globally, and will help to manage changes in the system.

Measurable outcome of success:

Success would be, for example, if long term comparison between Raman lidar water vapour measurements and another traceable reference measurement technique (e.g. GRUAN radiosondes) would be compared over long term showing a reduction in the lidar calibration uncertainty using absolute techniques as well as the added value of synergetic lidar-radiometer products during daytime operations. Evidences of this improvement have been reported in literature but comparisons over long time periods have not been reported yet.

Expected viability for the outcome of success:

- High

Scale of work:

- Individually
- Single institution
- Large consortium

Time bound to remedy:

- Less than 5 years

Indicative cost estimate (investment):

- Low cost (< 1 million)

Indicative cost estimate (exploitation):

Non-applicable

Potential actors:

- Academia, individual research institutes
- SMEs/industry
- National measurement institutes

References:

- Boers, R., van Meijgaard, E., 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.
- Weatherhead, E. C., and coauthors, Factors affecting the detection of trends: Statistical considerations and applications to environmental data. J. Geophys. Res., 103, 17 149–17 161, doi:10.1029/98JD00995, 1998.

G2.10 Tropospheric ozone profile data from non-satellite measurement sources is limited and improved capability is needed to characterise new satellite missions

Feedback

Gap abstract:

Tropospheric ozone has an impact on air quality and acts as a greenhouse gas and therefore plays a role in public and environmental health, as well as climate change, linking the two subjects. Establishing processes and trends in tropospheric ozone, in particular in the free troposphere, above the mixed layer and below the stratosphere, is difficult due to a lack of data. Also, ozone soundings using balloon borne samplers are too scarce to capture the relatively high spatial and temporal variability in the troposphere. Contrary to stratospheric ozone, passive satellite observations have limited access to information about tropospheric ozone. However, new sensors on the next generation of satellite measurements shall have better tropospheric sensing capabilities, and shall require validation.

Part I: Gap description

Primary gap type:

Spatiotemporal coverage

Secondary gap type:

Vertical domain and/or vertical resolution

ECVs impacted:

Ozone

User category/Application area impacted:

- Operational services and service development (meteorological services, environmental services, Copernicus Climate Change Service (C3S) and Atmospheric Monitoring Service (CAMS), operational data assimilation development, etc.)
- Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)

Non-satellite instrument techniques involved:

- Ozonesonde
- Lidar

Detailed description:

Tropospheric ozone has an impact on air quality and acts as a greenhouse gas and therefore plays a role in public and environmental health, as well as climate change, linking the two subjects. Establishing processes and trends in tropospheric ozone, in particular in the free troposphere, above the mixed layer and below the stratosphere, is difficult due to a lack of direct observational data. Tropospheric ozone is much more variable in space and time than stratospheric ozone due to transport and chemistry. The frequency and accuracy of the observations should ideally be adjusted to account for this elevated variability. In addition, the balloon borne ozone samplers are optimised for stratospheric observations, which implies sub optimal performance in the troposphere. Therefore, other observational techniques are required to fill the need for observations of tropospheric ozone from non-satellite sources that are more routinely operational. Contrary to stratospheric ozone, passive satellite observations have limited access to information about tropospheric ozone as the TOA down view is largely dominated by the much higher stratospheric loadings across the sensitive regions of the E-M spectrum. However, currently planned missions are envisaged to have better tropospheric ozone sensing capabilities. Also, ozone soundings using balloon borne samplers are too scarce to capture the relatively high spatial and temporal variability in the troposphere.

Operational space missions or space instruments impacted:

- Copernicus Sentinel 4/5
- MetOp
- MetOp-SG
- OMPS
- Polar orbiters
- Geostationary satellites
- UV/VIS nadir
- Passive sensors

Validation aspects addressed:

- Geophysical product (Level 2 product)
- Gridded product (Level 3)
- Assimilated product (Level 4)
- Time series and trends
- Representativity (spatial, temporal)
- Calibration (relative, absolute)

Gap status after GAIA-CLIM:

After GAIA-CLIM this gap remains unaddressed.

Part II: Benefits to resolution and risks to non-resolution

Identified benefit	User category/Application area benefitted	Probability of benefit being realised	Impacts
Upcoming satellite missions will have improved capabilities for tropospheric ozone. Sub-orbital observation capacity will be used to assess the satellite data quality.	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	Medium Low	Improved knowledge of tropospheric ozone will reduce uncertainty in radiative transfer (climate) and improve results for chemistry.
Identified risk	**User category/Application area benefitted**	**Probability of benefit being realised**	**Impacts**
Tropospheric ozone profile data is relatively scarce and limits applicability to range of activities including tropospheric ozone validation from satellites.	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Remaining gap in appropriate data sources to optimally use new satellite data and to understand processes in the troposphere related to the linkage between air pollution and climate change.

Part III: Gap remedies

Gap remedies:

Remedy 1: Expand coverage of differential absorption lidars to improve ability to characterise tropospheric ozone

Primary gap remedy type:

Deployment

Secondary gap remedy type:

Technical

Proposed remedy description:

An increase in data on tropospheric ozone is expected from various space-borne platforms with increased capabilities, such as OMPS, TES and TROPOMI and the instruments proposed for Sentinel 4 and 5. However, a reinforcement of the ground based observational capacity is also required to validate these space-borne observations and establish high-quality time series. An increase in the number of ozone balloon borne soundings is not likely due to the high costs involved (material and personnel). There is a potential for tropospheric ozone lidars (using the differential absorption lidar technique) to fill this gap. In the US, a network of tropospheric ozone lidars has been established (TOLNET). Similar initiatives could be pursued in Europe, where a latent tropospheric ozone lidar network could be revived. In Europe, such a network might become part of ACTRIS, the European Research Infrastructure which deals with short-lived greenhouse agents. Similar efforts are required in other areas of the globe to enable full characterisation of tropospheric ozone capabilities by future satellite missions.

Relevance:

An increase in data on tropospheric ozone is expected from various space-borne platforms with increased capabilities, such as OMPS, TES and TROPOMI and the instruments proposed for Sentinel 4 and 5. However, a reinforcement of the ground based observational capacity is also required to validate these space borne observations and establish high-quality time series. The issue is relevant to understand the links between air pollution and climate change. Satellite data alone will likely not suffice to fill the gap.

Measurable outcome of success:

A measure of success is the increase in the number of available tropospheric ozone profiles.

Expected viability for the outcome of success:

Medium

Scale of work:

Programmatic multi-year, multi-institution activity

Time bound to remedy:

Less than 3 years

Indicative cost estimate (investment):

High cost (> 5 million)

Indicative cost estimate (exploitation):

Yes

Potential actors:

- EU H2020 funding
- Copernicus funding
- National funding agencies
- National Meteorological Services
- WMO
- ESA, EUMETSAT or other space agency

G2.11 Lack of rigorous tropospheric ozone lidar error budget availability

Feedback

Gap abstract:

Tropospheric ozone has an impact on air quality and acts as a greenhouse gas and therefore plays a role in public and environmental health, as well as climate change, linking the two subjects. In order to establish tropospheric ozone trends, more high-quality and high-frequency observations are needed (see G.2.10) and a rigorous error budget is required. Measurements of tropospheric ozone by means of the Differential Absorption Lidar (DIAL) technique are close to reference quality and may meet this need if development of traceable products can be realised. The methodology of rigorous error-budget calculations is available, but needs to be implemented across available data sources.

Part I: Gap description

Primary gap type:

Implementation of uncertainty budget and calibration

ECVs impacted:

Ozone

User category/Application area impacted:

- Operational services and service development (meteorological services, environmental services, Copernicus Climate Change Service (C3S) and Atmospheric Monitoring Service (CAMS), operational data assimilation development, etc.)
- Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)

Non-satellite instrument techniques involved:

Lidar

Related gaps:

G2.10 Tropospheric ozone profile data from non-satellite measurement sources is limited and improved capability is needed to characterise new satellite missions

Gap 2.10 relates to the provision of more observations. Gap 2.11 should thus be addressed at the same time or after closing G2.10.

Detailed description:

Tropospheric ozone has an impact on air quality and acts as a greenhouse gas and therefore plays a role in public and environmental health, as well as climate change, linking the two subjects. In order to establish trends, more observations are needed (see G.2.10) and a rigorous error budget is needed for these observations to assure their quality. Tropospheric ozone profiles can be attained from lidar measurements (amongst others). Measurements of tropospheric ozone by means of the Differential Absorption Lidar (DIAL) technique are described in detail, metrologically characterised, and processed in a consistent comparable manner. Such data would greatly aid efforts at the characterisation of new and planned space missions which are envisaged to be capable of measuring tropospheric ozone changes and variability. Although these descriptions are now available, these should be more widely implemented across available data sources. In case of networked operation of tropospheric ozone DIAL instruments, this could be achieved by centralised data processing. However, not all available data sources are readily accessible and several rely on diverse, in-house developed processing and analysis techniques.

Operational space missions or space instruments impacted:

- Copernicus Sentinel 4/5
- Meteosat Third Generation (MTG)
- MetOp
- MetOp-SG
- OMPS
- Polar orbiters
- Geostationary satellites
- Passive sensors

Validation aspects addressed:

- Geophysical product (Level 2 product)
- Gridded product (Level 3)
- Assimilated product (Level 4)
- Time series and trends
- Representativity (spatial, temporal)
- Calibration (relative, absolute)

Gap status after GAIA-CLIM:

GAIA-CLIM has partly closed this gap:
GAIA-CLIM work on metrological characterisation has led to a partial resolution of this gap.

Part II: Benefits to resolution and risks to non-resolution

Identified benefit	User category/Application area benefitted	Probability of benefit being realised	Impacts
Upcoming satellite missions will have improved capabilities for tropospheric ozone. Data available from existing tropospheric ozone DIAL instruments will be traceable.	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Improved knowledge of tropospheric ozone will reduce uncertainty in radiative transfer (climate) and improve results for chemistry.
Identified risk	**User category/Application area benefitted**	**Probability of benefit being realised**	**Impacts**
Lack of rigorous tropospheric O3 lidar error budget availability	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Reduced level of traceability of tropospheric ozone lidar measurements leading to ambiguity in downstream applications such as satellite cal/val.

Part III: Gap remedies

Gap remedies:

Remedy 1: Create and disseminate a fully traceable reference-quality DIAL lidar product

Primary gap remedy type:

Deployment

Secondary gap remedy type:

- Technical
- Research
- Education/Training

Proposed remedy description:

Work has been undertaken to attain a fully traceable product for the DIAL lidar technique to measure tropospheric ozone profile data. A traceability chain has been fully documented. The uncertainty in each step in the processing chain has been quantified in a robust manner. Documentation as to how to undertake such traceable measurements has been published in the peer reviewed literature. Now these methods and calculations need to be implemented across potential networks and individual stations. This requires funding support to networks and individual sites to enable measurements to be undertaken in a comparable manner. It also requires support for centralised processing, archival and dissemination.

Relevance:

The issue is highly relevant for any application that uses ground based tropospheric ozone lidar data as a reference. In particular to understand the tropospheric ozone budget and the reduction of the uncertainties in estimation of the resulting radiative forcing.

Measurable outcome of success:

Established (published in peer reviewed journal) error budget calculation scheme.

Expected viability for the outcome of success:

High

Scale of work:

Single institution
Consortium

Time bound to remedy:

Less than 1 year

Indicative cost estimate (investment):

Low cost (< 1 million)

Indicative cost estimate (exploitation):

Yes, ongoing annual costs to maintain (low)

Potential actors:

- EU H2020 funding
- Copernicus funding
- National funding agencies
- National Meteorological Services
- WMO
- ESA, EUMETSAT or other space agency

G2.12 Lack of rigorous pure rotational Raman temperature lidar error budget availability limits utility for applications such as satellite characterisation

Feedback

Gap abstract:

Temperature lidars provide important information for trend detection in the middle atmosphere (connected to trends in the ozone layer). These are measured using lidar systems that often also measure the ozone layer. The lidar technique to measure temperature is sensitive to the presence of aerosol, which is an important contribution to the error budget. In addition, lidar techniques exist to measure temperature profiles in the troposphere using the pure-rotational Raman (PRR) technique that can be used in the presence of aerosol. For temperature measurements in the presence of aerosols using the PRR technique, a rigorous error budget needs to be established to improve their utility for applications such as satellite characterisation.

Part I: Gap description

Primary gap type:

Knowledge of uncertainty budget and calibration

ECVs impacted:

Temperature

User category/Application area impacted:

- Operational services and service development (meteorological services, environmental services, Copernicus Climate Change Service (C3S) and Atmospheric Monitoring Service (CAMS), operational data assimilation development, etc.)
- Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)

Non-satellite instrument techniques involved:

Lidar

Detailed description:

Temperature lidars provide important information for trend detection in the middle atmosphere (connected to trends in the ozone layer). The temperature profiles in the middle atmosphere (12- 80 km altitude) are measured using lidar systems that often also measure the ozone layer. The temperature measurements are done using the

Rayleigh-Mie technique. This lidar technique to measure temperature is sensitive to the presence of aerosol, which is an important contribution to the error budget. An additional lidar technique exists to measure temperature profile (in the troposphere) using the pure-rotational Raman technique (PRR) that can be used in the presence of aerosol. However, presently a metrologically traceable processing is unavailable for such measurements. Hence, for temperature measurements in the presence of aerosols using the PRR lidar technique, a rigorous error budget needs to be established to improve their utility for applications such as satellite characterization.

Operational space missions or space instruments impacted:

Independent of specific space mission or space instruments

Validation aspects addressed:

Time series and trends
Auxiliary parameters (clouds, lightpath, surface albedo, emissivity)

Gap status after GAIA-CLIM:

After GAIA-CLIM, this gap remains unaddressed.

Part II: Benefits to resolution and risks to non-resolution

Identified benefit	**User category/Application area benefitted**	**Probability of benefit being realised**	**Impacts**
A traceable error budget for PRR temperature lidar will become available in addition to the existing RM temperature lidar used for the establishment of time series	Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Better climate records will become available.
A traceable error PRR lidar budget will become available for the comparison to other techniques for temperature profile measurements.	Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Redundancy in time series will improve confidence in data records.
PRR lidar error budgets will become available for users of data as auxiliary input.	Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Improved uncertainty budgets for products relying on auxiliary input from lidar temperature profiles.

Identified risk	User category/Application area benefitted	Probability of benefit being realised	Impacts
Lack of rigorous temperature PRR lidar error budget availability	Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Reduced level of traceability of temperature lidar measurements leading to ambiguity in subsequent applications such as satellite Cal/Val.

Part III: Gap remedies

Gap remedies:

Remedy 1 Create a fully traceable reference-quality temperature lidar product

Primary gap remedy type:

Research

Secondary gap remedy type:

- Technical
- Deployment
- Education/Training

Proposed remedy description:

The existing traceability chain for temperature lidar measurements will need to be expanded with the necessary elements for the temperature measurements with the pure rotational Raman Lidar technique. The chain will describe all the processing steps in the PRR temperature lidar measurement system. Robust estimation of uncertainties shall be undertaken that appropriately codifies the knowledge of each step and its resultant uncertainty. These uncertainties shall be used to derive an error budget calculation scheme which will be compiled. It shall be accompanied by detailed documentation of the measurement technique, the instrumental aspects, the processing steps and auxiliary input to the algorithms. These results shall be published via the peer reviewed literature. Processing shall be enacted such that products meeting the detailed procedures are available for end-users.

Relevance:

The issue is highly relevant for any application that uses ground based temperature lidar data as input or reference. In particular, to detect temperature trends in the middle atmosphere and aerosol-cloud-humidity interactions.

Measurable outcome of success:

Established (published in peer reviewed journal) error budget calculation scheme that includes detailed documentation of the measurement technique, the instrumental aspects, the processing steps and auxiliary input to the algorithms.

Expected viability for the outcome of success:

High

Scale of work:

Consortium

Time bound to remedy:

Less than 2 years

Indicative cost estimate (investment):

Low cost (< 1 million)

Indicative cost estimate (exploitation):

No

Potential actors:

- EU H2020 funding
- Copernicus funding
- National funding agencies
- National Meteorological Services
- WMO
- ESA, EUMETSAT or other space agency

G2.13 Missing microwave standards maintained by national/international measurement institutes

Gap abstract:

The traceability of ground-based microwave radiometer (MWR) estimates and their uncertainty requires the traceability of MWR calibration to SI standards. Currently, no SI standard is available for MWR at any national/international measurement institute. Thus, full SI-traceability of ECVs from MWR is currently not feasible. However, at least one national measurement institute is currently developing SI standards for MWR. It is expected that SI-traceable standards for MWR will be available in the next few years. This will then allow the availability of transfer standards to MWR manufacturer and user communities.

Part I: Gap description

Primary gap type:

Knowledge of uncertainty budget and calibration

Secondary gap type:

Uncertainty in relation to comparator measures
Governance (missing documentation, cooperation etc.)

ECVs impacted:

- Temperature
- Water vapour

User category/Application area impacted:

- Operational services and service development (meteorological services, environmental services, Copernicus Climate Change Service (C3S) and Atmospheric Monitoring Service (CAMS), operational data assimilation development, etc.)
- Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)

Non-satellite instrument techniques involved:

Microwave Radiometer

Related gaps:

- G2.36 Lack of traceable uncertainties in MWR measurements and retrievals

G2.13 should be addressed together with G2.36

The remedy of G2.13, i.e. the development of MW standards maintained at national/international measurement institutes and the availability of transfer standards, will set the basis for SI-traceability of MWR observations and retrievals. However, tools for evaluating the MWR total uncertainty budget can be developed independently of the solution of G2.13.

Detailed description:

The traceability of the microwave radiometer (MWR) estimates and their uncertainty requires the traceability of MWR calibration to SI standards. This implies the use of certified black-body (BB) targets and temperature sensors (measuring the target physical temperature). Commercial BB targets have reached a mature state, but their characterization is usually limited. Despite this, many realizations of microwave brightness temperature standards exist in the form of heated or cooled calibration targets, although none are currently maintained as a standard by a national/international measurement institute (Walker, 2011). Thus, despite the efforts for fully characterizing the MWR absolute calibration, the traceability of any ECVs from MWR to national/international standards is currently not feasible. However, the development is ongoing (Houtz et al., 2015; 2016; 2017). This gap shall be addressed by national/international measurement institutes, and cannot be addressed within GAIA-CLIM.

Operational space missions or space instruments impacted:

Microwave and Infrared temperature and humidity sounders

Validation aspects addressed:

- Radiance (Level 1 product)
- Geophysical product (Level 2 product)
- Gridded product (Level 3)
- Assimilated product (Level 4)
- Time series and trends
- Calibration (relative, absolute)
- Spectroscopy

Status after GAIA-CLIM:

GAIA-CLIM has partly closed this gap:

This gap will be considered closed when MW standards are available in at least one national/international measurement institute for calibrating secondary standards to be used for MWR calibration. The role of GAIA-CLIM is to follow and report the technological developments at national/international measurement institutes (e.g. NIST) and to inform MWR users and manufacturers about these developments.

Part II: Benefits to resolution and risks to non-resolution

Identified benefit	User category/Application area benefitted	Probability of benefit being realised	Impacts
Traceable intra- and inter-MWR data characterization	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Traceable MWR characterization will allow proper reconciliation of historical time series of MWR observations at any given site as well as uniformly across the network
Increased confidence in MWR data quality	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Traceable MWR data characterization will yield increased confidence and utilization of MWR observations in reanalyses and climate research
Identified risk	**User category/Application area benefitted**	**Probability of benefit being realised**	**Impacts**
Non-traceable MWR-based validation for satellite ECVs	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Difficult to reconcile historical time series of MWR observations. Ground-based MWR will not reach the requirements for climate monitoring
Non-traceable MWR-based validation for satellite ECVs	All users and application areas will suffer from it.	High	No traceable validation for satellite boundary layer thermodynamical profiles

Part III: Gap remedies

Gap remedies:

Remedy 1: Development and testing of MWR standards and secondary standards

Primary gap remedy type:

Technical
TRL 4-6

Secondary gap remedy type:

- Laboratory
- Deployment
- Research

Proposed remedy description:

Metrology applicable to microwave remote sensing radiometry is currently under development at national/international measurement institutes (e.g. National Institute for Standards and Technology, USA). These efforts include the development of a standard radiometer and standard high-emissivity black body (BB) targets. It is expected that SI-traceable calibration for BB targets and transfer standards in the form of calibrated BB targets will be available at NIST in the next few years. The current status is presented in an open literature paper (Houtz et al., 2017). The uncertainty in the BB Tb is around 0.1 K (1-sigma), covering the frequency range from 10 to 200 GHz. NIST plans to be able to calibrate other BB targets against their standards, which could then be used as transfer standards. Thus, the primary gap remedy type is technical/technological (the development of MW standards), but it involves laboratory and research work (testing and characterization) as well as deployment (transfer standard to manufacturer and user communities).

Relevance:

The remedy will make microwave standards available at least at one measurement institute (NIST). GAIA-CLIM aims at monitoring and effectively communicating the progress to MWR manufacturers and users, in order to promote the uptake of certified targets.

Measurable outcome of success:

The successful outcome is to make MWR users and manufacturers aware of the above developments. The effective characterization of existing and/or new MWR units against microwave standards would be an additional measure of success, which is subject to the availability of the transfer standards before the end of GAIA-CLIM.

Expected viability for the outcome of success:

Medium

Scale of work:

Single institution

Time bound to remedy:

Less than 5 years

Indicative cost estimate (investment):

Medium cost (< 5 million)

Indicative cost estimate (exploitation):

Yes

Potential actors:

- Academia, individual research institutes
- SMEs/industry
- National measurement institutes

References:

- Houtz D. A., D. K. Walker and D. Gu, Simulations to characterize a passive microwave blackbody design, 2015 IEEE International Geoscience and Remote Sensing Symposium (IGARSS), Milan, pp. 3485-3488, DOI: 10.1109/IGARSS.2015.7326571, 2015.
- Houtz D. A., D. K. Walker, D. Gu (2016), Cryogenic Design and Uncertainty Analysis of the NIST Microwave Blackbody, 14th Specialist Meeting on Microwave Radiometry and Remote Sensing of the Environment (MicroRad), Espoo, Finland, April 11-14, 2016.
- Houtz D. A., W. Emery, D. Gu, K. Jacob, A. Murk, D. K. Walker, and R. J. Wylde, Electromagnetic Design and Performance of a Conical Microwave Blackbody Target for Radiometer Calibration, IEEE Transactions on Geoscience and Remote Sensing, vol. 55, no. 8, pp. 4586-4596, doi: 10.1109/TGRS.2017.2694319, Aug. 2017.
- Walker D. K., Microwave radiometric standards development at US NIST, IEEE GRSS Newsletter, 161, 2011.

G2.18 Better agreement needed on systematic and random components of the uncertainty in FTIR measurements and how to evaluate them

Gap abstract:

There is no clear agreement yet within the FTIR community on the distinction and characterisation of the random and systematic components of the uncertainty in FTIR measurements. As a consequence, no common approach is available on how to evaluate these components appropriately leading to a degree of heterogeneity in the global FTIR network.

Part I: Gap description

Primary gap type:

Knowledge of uncertainty budget and calibration

Secondary gap type:

Technical (missing tools, formats etc.)

ECVs impacted:

- Water vapour
- Ozone
- Aerosols
- Carbon Dioxide
- Methane

User category/Application area impacted:

- Operational services and service development (meteorological services, environmental services, Copernicus Climate Change Service (C3S) and Atmospheric Monitoring Service (CAMS), operational data assimilation development, etc.)
- International (collaborative) frameworks and bodies (SDGs, space agencies, EU institutions, WMO programmes/frameworks etc.)
- Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)

Non-satellite instrument techniques involved:

FTIR

Related gaps:

- G2.37 Poorly quantified uncertainties in spectroscopic information
- G3.04 Limited characterization of the multi-dimensional (spatiotemporal) smoothing and sampling properties of atmospheric remote sensing systems, and of the resulting uncertainties
- G2.22 FTIR cell measurements carried out to characterize ILS have their own uncertainties

All these gaps deal with the characterisation of the data quality of FTIR. Thus, they should all be considered at the same time as or prior to the resolution of the current gap.

Detailed description:

Within the NDACC FTIR working group, the technical implementation of the uncertainty propagation (both random and systematic) is fully achieved within the EU QA4ECV and GAIA-CLIM projects. However, each PI must determine a good estimate of site-specific uncertainties on the parameters used as input to the retrieval setup. During the QA4ECV and GAIA-CLIM projects, it was observed that there is not full agreement within the FTIR working group on how the estimation of random and systematic uncertainties for these input parameters should be done. Also, there is no full agreement across the two main retrieval software packages SFIT4 and PROFFIT. Random and systematic uncertainty sources are often assumed differently for different sites/different retrieval software. Although the current data products generated during the QA4ECV and GAIA-CLIM projects are highly harmonzied across participating sites, the network will benefit from a further harmonisation of the uncertainty source assumption. A clear distinction between systematic and random uncertainties implemented network-wide, is important for determining accuracy and precision, e.g. when comparing to satellite data, and uncertainty of an average of data.

Operational space missions or space instruments impacted:

Independent of specific space mission or space instruments

Validation aspects addressed:

Geophysical product (Level 2 product)

Gap status after GAIA-CLIM:

GAIA-CLIM has partly closed this gap.

Recipes to evaluate random and systematic parts of the uncertainty sources will be promoted, but that does not mean yet that they will be implemented at each FTIR site by the end of GAIA-CLIM.

Part II: Benefits to resolution and risks to non-resolution

Identified benefit	User category/Application area benefitted	Probability of benefit being realised	Impacts
Traceable and consistent error characterization of the FTIR data products	International (collaboration) frameworks (SDGs, space agency, EU institutions, WMO programmes/frameworks etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	The agreement on the input data for the uncertainty calculations will assure that the error estimations are consistently traceable and comparable between different sites.
Identified risk	**User category/Application area benefitted**	**Probability of benefit being realised**	**Impacts**
Incomparable uncertainty budgets for different sites within NDACC.	International (collaboration) frameworks (SDGs, space agency, EU institutions, WMO programmes/frameworks etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Difficulty of a network-wide and consistent data usage by downstream applications that require network homogeneity.

Part III: Gap remedies

Gap remedies:

Remedy 1: Improved traceability of uncertainties in FTIR measurements

Primary gap remedy type:

Technical

Secondary gap remedy type:

Education/Training

Proposed remedy description:

Comparison and tuning of the uncertainty modules of the retrieval software packages. Write down a manual of how to estimate the uncertainties for all parameters that are part of the forward model in the retrieval software packages.

Further, a recipe should be developed as to how a random and systematic uncertainty should be determined for each of the leading uncertainty contributions and this recipe should be promoted and implemented in both retrieval software packages at all NDACC FTIR sites. Ideally a centralized QC system or processing will remedy the online publication of FTIR data whose uncertainty budgets is not compliant with the proposed guidelines.

Relevance:

Improved traceability of errors is a core objective of GAIA-CLIM. Traceable ILS uncertainty will allow a traceable estimation of the FTIR product uncertainty due to ILS uncertainties.

Measurable outcome of success:

Comparable and consistently traceable errors for all different sites.

Expected viability for the outcome of success:

High

Scale of work:

Consortium

Time bound to remedy:

Less than 1 year

Indicative cost estimate (investment):

Low cost (< 1 million)

Indicative cost Estimate (exploitation):

No

Potential actors:

Academia, individual research institutes

G2.22 FTIR cell measurements carried out to characterize Instrument Line Shape have their own uncertainties

Gap abstract:

For the retrieval of information about the vertical distribution of target species from FTIR spectra, it is important to know the FTIR instrument line shape (ILS). Therefore, regular cell measurements are carried out to characterize the ILS of the FTIR spectrometers. However, these cell measurements have their own uncertainties since these are obtained using optimal estimation: an ILS retrieval comes along with an uncertainty and an averaging kernel. In particular the averaging kernel for an ILS retrieval is often not adequately considered (Hase, 2012). Inaccurate knowledge of the ILS mainly affects the retrieved vertical profile (e.g. for water vapour and ozone profile retrievals). The uncertainty on the ILS leads to larger uncertainties on the retrieved column-averaged concentrations of CH_4 and CO_2 (XCH_4, XCO_2). In other words, the uncertainties on the ILS retrieved from cell measurements will propagate to the total uncertainty budget of the retrieved species. Although the technical know-how is present within the NDACC IR working group, the actual implementation of the ILS uncertainty characterisation and propagation is not complete. In particular further harmonization between the different FTIR retrieval software packages is required.

Part I: Gap description

Primary gap type:

Knowledge of uncertainty budget and calibration

ECVs impacted:

- Water vapour
- Ozone
- Carbon Dioxide
- Methane

User category/Application area impacted:

- Operational services and service development (meteorological services, environmental services, Copernicus Climate Change Service (C3S) and Atmospheric Monitoring Service (CAMS), operational data assimilation development, etc.)
- International (collaborative) frameworks and bodies (SDGs, space agencies, EU institutions, WMO programmes/frameworks etc.)
- Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)

Non-satellite instrument techniques involved:

FTIR

Related gaps:

G2.18 Better agreement needed on systematic and random part of the uncertainty in FTIR measurements and how to evaluate each part
This gap should be considered at the same time as G2.18 as it is a contributing component to the broader uncertainty characterisation.

Detailed description:

The retrieval of vertical profile information for target gases from ground-based high-spectral-resolution FTIR solar absorption spectra is based on the analysis of the observed shape(s) of the absorption line(s) of the target species in the recorded spectra. Since the observed shape is a convolution of the intrinsic absorption line shape with the instrument line shape (ILS), the analysis must account for the ILS. Therefore, the ILS must be known highly accurately. To this end, a cell filled with a known gas concentration at a known temperature and pressure is put into the FTIR instrument and a spectrum of the cell gas is taken. The cell spectrum allows the retrieval of the ILS using optimal estimation as described by Rodgers (2000), and such a retrieved ILS comes with its uncertainty. The uncertainty on the retrieved ILS is a combination of the smoothing uncertainty, the noise, the forward model parameters, etc. This uncertainty will propagate into the total uncertainty budget of the retrieved target gas′ profile and total abundance.

In summary, one can state that the cell measurement serves as a calibration of the target gas retrieval but that this calibration method is itself indebted with some uncertainty that must be accounted for in the total uncertainty budget of the retrieval result, which is the target gas vertical profile and total abundance.

Operational space missions or space instruments impacted:

- Copernicus Sentinel 4/5
- MetOp
- MetOp-SG
- Polar orbiters
- Geostationary satellites
- Infrared nadir
- Other:
  All missions/instruments that use ground-based FTIR data for validation

Validation aspects addressed:

Geophysical product (Level 2 product)

Gap status after GAIA-CLIM:

GAIA-CLIM has partly closed this gap:

Progress has been made within GAIA-CLIM, to identify the contribution of the ILS uncertainty to the total uncertainty budget and to make it better traceable and better characterised. The uncertainty propagation routines that were developed during QA4ECV & GAIA-CLIM are such that the integration of the ILS uncertainty propagation is a straightforward extension. However, the harmonization between the different retrieval software packages is not complete yet, and the implementation at all FTIR stations should still be done consistently.

Part II: Benefits to resolution and risks to non-resolution

Identified benefit	User category/Application area benefitted	Probability of benefit being realised	Impacts
Better uncertainty characterization of the FTIR data products	All users and application areas will benefit from it	High	Better characterized ground-based FTIR data yield improved utilization as reference data
Identified risk	**User category/Application area benefitted**	**Probability of benefit being realised**	**Impacts**
Missing contribution to total uncertainty budget of the ground-based FTIR data products	All users and application areas will suffer from it.	High	Underestimation of total uncertainty associated with ground-based FTIR data products.
Inconsistent characterisation of FTIR data between different NDACC sites (not at all stations the quality of the cell retrievals is analysed in the same manner)	All users and application areas will suffer from it.	High	Reduced confidence in network wide data consistency.

Part III: Gap remedies

Gap remedies:

Remedy 1: Regular cell measurements and ILS retrievals are to be performed in a consistent manner

Primary gap remedy type:

Technical

TRL6

Secondary gap remedy type:

Education/Training

Proposed remedy description:

Regular cell measurements have to be performed at all NDACC sites and ILS retrievals have to be performed in a consistent manner regarding both, the technical setup of the retrieval (regularization, retrieval paramaters, cell measurement setup etc.) as well as the calculation of the total random and systematic uncertainty on the retrieved ILS. Ideally, the random and systematic uncertainties on the retrieved ILS are expressed as full uncertainty covariance matrix, but it is unrealistic and a computational burden to determine and propagate such full covariance matrices. A good approach would be to characterise the leading ILS uncertainty contributions, smoothing/noise, random/systematic and accordingly work on a realistic and not oversimplifying approach to accurately estimate and propagate the ILS uncertainties towards the retrieved target gas.

The second step in the proposal would be to implement this ILS uncertainty characterisation in both existing retrieval software packages PROFFIT and SFIT4. The outcome is a FTIR NDACC network-wide harmonized uncertainty budget that includes the propagated ILS uncertainty.

Relevance:

Improved traceability of uncertainties is a core objective of GAIA-CLIM and shall benefit applications including but not limited to satellite characterisation by FTIR instruments.

Measurable outcome of success:

Traceable ILS uncertainty will allow a traceable estimation of the FTIR product uncertainty due to ILS uncertainties.

Expected viability for the outcome of success:

High

Scale of work:

Consortium

Time bound to remedy:

Less than 3 years

Indicative cost estimate (investment):

Low cost (< 1 million)

Indicative cost estimate (exploitation):

Yes

Potential actors:

Academia, individual research institutes

References:

- 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.
- Rodgers, C. D., Inverse Methods for Atmospheric Sounding: Theory and Practice, Ser. Atmos. Oceanic Planet. Phys., Vol. 2, 1st ed., World Sci., Hackensack, N. J., 2000.

G2.24 Lack of calibrated in-situ vertical profiles of CH_4, CO_2 (and CO) for improving the accuracy of FTIR (partial) column measurements of CH_4, CO_2 (and CO)

Gap abstract:

This gap addresses the need for sustained calibration of the FTIR remote sensing data (essentially columns with some vertical information that enables to separate partial columns) for CO_2, CH_4 (and CO). This can be done by comparing the FTIR data with co-located or nearby in-situ soundings of the same species that are calibrated to community standards, in this case the WMO standards. At present, however, there is not enough capacity to provide such in-situ data.

This gap also addresses the need for a European infrastructure for vertical greenhouse gas profiling in the troposphere for CO_2 and CH_4 There is a need for vertical profile information about these ECVs in the troposphere, among others, to verify model results, and to validate remote sensing total and partial column data. The capabilities of the ground-based remote-sensing observing systems are limited when it comes to vertical-profile information, and are not sufficiently validated. Options for filling this gap are the facilitation of access to airborne in-situ measurement systems, like aircraft or UAV, or Aircore for greenhouse gases.

Part I Gap description

Primary gap type:

Knowledge of uncertainty budget and calibration

Secondary gap type:

- Spatiotemporal coverage
- Vertical domain and/or vertical resolution
- Technical

ECVs impacted:

- Carbon Dioxide
- Methane

User category/Application area impacted:

- Operational services and service development (meteorological services, environmental services, Copernicus Climate Change Service (C3S) and Atmospheric Monitoring Service (CAMS), operational data assimilation development, etc.)

- International (collaborative) frameworks and bodies (SDGs, space agencies, EU institutions, WMO programmes/frameworks etc.)

- Climate research *(research groups working on development, validation and improvement of ECV Climate Data Records)*

Non-satellite instrument techniques involved:

FTIR

Detailed description:

For the ECVs temperature, ozone, water vapour and aerosol, vertical-profile information with relatively high vertical resolution (100m to a few km) in the troposphere is available from sonde and/or lidar measurements. For greenhouse gases (CO, CH_4, CO_2), the non-satellite observing system does not have sufficient capabilities. The FTIR measurements of these greenhouse gases have a low vertical resolution of the order of 5 to 8 km, if any, and this vertical information is difficult to validate. For example, measurements analysed so far within the GAIA-CLIM project have shown that the CH_4 retrieval can be improved under polar vortex conditions as a result of applying new profile data. Also, the modelling component in GAIA-CLIM has highlighted the deficiencies of the FTIR vertical profile information and the resulting needs for better in-situ vertical profiles.

One option to obtain in-situ vertical profiles is the use of the Aircore technique. This technique has been under development since 2000 and has the capability to obtain vertical profiles up to the middle stratosphere. Several Aircore sites exist in Europe, but the system is not yet a fully operational system. It is necessary to make the Aircore measurements easier for the users. Moreover, the Aircore cannot be launched at all sites, due to air traffic limitations and the fact that the Aircore must be recovered upon landing. The landing site cannot be pre-determined as long as the Aircore is launched with a balloon and descends with a simple parachute, thereby drifting with the wind and landing at a location which is not always suitable for retrieving the payload for performing the post-flight analysis of the air sample.

To solve the latter issue, some projects have investigated the design of a steered system to bring the Aircore down. A second option to obtain in-situ vertical profiles of greenhouse gases is to make use of aircraft spiral flights. The aircraft capacity in Europe is too limited to perform regular aircraft campaigns. Europe has no capability similar to the HIPPO campaigns in the USA. In any case, aircraft campaigns cannot cover vertical profiles higher than 12 km (a better calibration is possible if the profiles cover an altitude range from the ground up to the middle stratosphere), are very expensive, and are also difficult to organise above remote locations that are not situated on the European continent. High-altitude UAV or Aircore are required to cover higher altitudes. At present, high-altitude UAV are still largely in proof-of-concept stage.

However, although expensive, in-situ calibration of CH_4, CO_2 (and CO) columns/profiles measured by FTIR remote sensing instruments can be performed by aircraft overpasses equipped with in-situ instruments that are calibrated relative to the WMO standards. Such campaigns have been undertaken in the past, for example in Europe as part of the EU project IMECC. But, as mentioned above, new flight campaigns in Europe are currently not planned, the flights cover only an altitude up to about 12 km, and calibration flights are very costly and difficult over stations that are not situated in the European continent, like islands, S. America, Africa, Asia. Hence more regular verification of the calibration of the instruments is desirable, to ensure long-term and network-wide consistency with the

standards, as well as to ensure a better understanding and minimization of the biases across the networks when studying fluxes from e.g. hot spot regions.

Operational space missions or space instruments impacted:

Current and future satellite missions, which have the capability to measure greenhouse gases from space include GOSAT, IASI, OCO-2, Tansat, S5P, GOSAT-2, Merlin, MicroCarb, OCO-3, Sentinel-5.

Validation aspects addressed:

Geophysical product (Level 2 product)

Gap status after GAIA-CLIM:

After GAIA-CLIM, this gap will remain.

New Aircore in-situ vertical profile data will be made available outside of GAIA-CLIM that can serve as calibration of FTIR greenhouse gas measurements and in support of modelling activities. However, they are limited to only one site (Sodankyla) and with limited temporal coverage.

Part II Benefits to resolution and risks to non-resolution

Identified benefit	User category/Application area benefitted	Probability of benefit being realised	Impacts
Increased accuracy of the measurements by ground-based network for validation/calibration purposes	International (collaboration) frameworks (SDGs, space agency, EU institutions, WMO programmes/frameworks etc.)	High	Increases confidence in space borne measurements
Increased intra-network and inter-network (e.g., TCCON with ICOS) consistency	International (collaboration) frameworks (SDGs, space agency, EU institutions, WMO programmes/frameworks etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Use of all network data without inconsistencies will increase the number of reliable data available for applications like flux inversions
Improved retrieval algorithms to be used by the sites	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.)	High	Retrieval algorithms will be improved, leading to better precision and accuracy of the measurements

	International (collaboration) frameworks (SDGs, space agency, EU institutions, WMO programmes/frameworks etc.)		
Identified risk	**User category/Application area benefitted**	**Probability of occurrence if gap not remedied**	**Impacts**
Inconsistencies in the network of FTIR data for the validation of satellite data	International (collaboration) frameworks (SDGs, space agency, EU institutions, WMO programmes/frameworks etc.)	Medium	Reliable global validation of GHG satellites is at risk
Lack of traceability of remote sensing data leading to possible inconsistencies between remote sensing data and in-situ data due to erroneous or no calibration of remote sensing data	Copernicus programme ICOS	High	Possible benefits of synergic exploitation of in-situ and remote sensing data are lost; the ICOS internal consistency is at risk
Significant uncertainties about vertical distribution of GHG in the troposphere	International (collaboration) frameworks (SDGs, space agency, EU institutions, WMO programmes/frameworks etc.)	High	Absence of data for verification/validation of models and satellite data, and of FTIR retrievals of vertical profile information of GHG

Part III Gap remedies

Gap remedies:

Remedy1: Operationalise the Aircore technique at a range of sites also measuring using FTIR

Primary gap remedy type:

Technical

Secondary gap remedy type:

Deployment

Proposed remedy description:

Currently, there is a limited availability of Aircore in Europe: only a few institutes have the required expertise to build and operate them, and to analyse the data. Moreover, the deployment of an Aircore depends on the availability of a suitable balloon launching site.

To enable operational use of the Aircore for providing vertical profiles of greenhouse gases over Europe and elsewhere on a regular basis, we need to have an Aircore system that is available 'off-the-shelf' and that can be used at many sites by non-expert users. Or we need a dedicated provider of Aircore data in Europe.

Moreover, we need an Aircore system that can be launched at many more sites, without meeting too many constraints about the site's environment. More specifically, we need an Aircore system that can descend in a steered way to a pre-determined landing site, and that complies with air traffic regulations. Currently, carrier platforms are being studied for bringing the Aircore down to a pre-defined landing spot, based on the concept of a steerable glider or Unmanned Airborne Vehicle (UAV). The development of this kind of system should be further extended and such systems should become readily available to the community.

Relevance:

The database of vertical profiles of greenhouse gases measured by Aircore will be used by the scientific community for verification and validation purposes, and for better calibration of the non-satellite and satellite remote sensing observing system to WMO standards (traceability). In the end, it will result in more reliable greenhouse gases products and trends, e.g., in Copernicus.

The remedy will also contribute to the network-wide, more cost-effective calibration tool.

Measurable outcome of success:

A much larger database of vertical profiles of greenhouse gases, with a better spatiotemporal spread.

Expected viability for the outcome of success:

High

Scale of work:

Consortium
Programmatic multi-year, multi-institution activity

Time bound to remedy:

Less than 3 years

Indicative cost estimate (investment):

Medium cost (< 5 million)

Potential actors:

- EU H2020 funding
- Copernicus funding
- WMO
- ESA, EUMETSAT or other space agency
- Academia, individual research institutes
- SMEs/industry

Remedy 2: Enhance the airborne infrastructure in Europe.

Primary gap remedy type:

Deployment

Secondary gap remedy type:

Technical

Proposed remedy description:

Currently there is a limited availability of suitable aircraft in Europe that can carry in-situ analysers of greenhouse gases to high altitude and make spiral flights to obtain vertical profiles. High-altitude UAV are still under development, but at the proof-of-concept phase and may have air traffic control restrictions that prove prohibitive.

We need an infrastructure and associated deployment programme that makes regular flights, especially over Europe but also over observation sites in other continents and the oceans, to obtain a good spatiotemporal sampling of the vertical distribution of greenhouse gases. This infrastructure can consist of aircrafts and/or UAV that can reach to high altitude. The scientific community should have easy access to this infrastructure for dedicated campaigns.

One option to realise this infrastructure is to engage more commercial airlines in the IAGOS RI such as to obtain a better spatiotemporal coverage of the profiles that are measured during take-off and landing of the aircrafts at the airports. Unfortunately, airports may not be representative for the background vertical profiles.

Relevance:

Such an aircraft / UAV fleet will be very useful also for other research purposes (e.g., T/ H_2O observations in the UTLS).

Measurable outcomes of success:

1. A much larger database of vertical profiles of greenhouse gases, with a better spatiotemporal spread. It will be used by the scientific community for verification and validation purposes, and for better calibration

of the non-satellite and satellite remote sensing observing system to WMO standards (traceability). In the end, it will result in more reliable greenhouse gases products and trends, e.g., in Copernicus.

2. Better competitiveness with the US airborne capabilities

Expected viability for the outcome of success:

High

Scale of work:

Programmatic multi-year, multi-institution activity

Time bound to remedy:

Less than 10 years

Indicative cost estimate (investment):

High cost (> 5 million)

Potential actors:

- EU H2020 funding
- Copernicus funding
- ESA, EUMETSAT or other space agency

Remedy 3: Create a database of in-situ vertical profiles of CO_2, CH_4, and CO with sufficient spatiotemporal coverage, possibly as part of the ICOS RI.

Primary gap remedy type:

Deployment

Secondary gap remedy type:

Governance

Proposed remedy description:

To enable a regular and network-wide calibration of remote sensing measurements (ground-based FTIR), the community needs access to a database of in-situ vertical profiles from regular airborne observations at different locations in Europe and beyond – in which the in-situ observations are calibrated against a commonly adopted standard (e.g., the WMO standard). This requires a sufficient capacity of well-calibrated airborne sensors and sufficient spiral flight opportunities close to the ground-based FTIR observatories (see remedies 1 and 2) from which to constitute such a database. In fact, this capacity should be part of the ICOS Research Infrastructure, to make it sustainable and fulfil the specific needs of the ICOS and ICOS-user communities. Hence, the proposed remedy is to create a database of in-situ vertical profiles of CO_2, CH_4 and CO with sufficient spatiotemporal coverage to calibrate FTIR profile information.

Relevance:

The remedy will contribute to the network-wide, more cost-effective calibration- making it consistent with the in-situ networks. This is very relevant for the ICOS RI and the Copernicus services (CAMS and C3S).

Measurable outcome of success:

The availability of an increased number of calibrated, in-situ vertical profile data of greenhouse gases with good spatiotemporal coverage would contribute to the next, improved version of the FTIR retrievals and to a better assessment of the seasonal cycle. It will lower the biases between sites in the network, and improve the consistency with surface in-situ measurements of the greenhouse gases as carried out in ICOS.

Expected viability for the outcome of success:

High, as soon as the database exists

Scale of work:

Consortium

Time bound to remedy:

Less than 5 years

Indicative cost estimate (investment):

Medium cost (< 5 million)

Potential actors:

- EU H2020 funding
- Copernicus funding
- National funding agencies
- WMO

- ESA, EUMETSAT or other space agency
- Academia, individual research institutes
- National measurement institutes

G2.26 Poorly understood uncertainty in ozone cross-sections used in the spectral fit for DOAS, MAX-DOAS and Pandora data analysis

Gap abstract:

The uncertainty in the ozone absorption cross-sections is one of the main systematic error sources in the remote sensing of atmospheric ozone using UV-visible spectroscopy techniques. It is a structured random effect in that even though the uncertainty can be considered as primarily a systematic error source, the actual error is dependent on atmospheric temperature which varies across the annual cycle and with synoptic conditions. Presently the uncertainty in total column ozone due to uncertainty in absorption cross-sections is assumed to be around one to a few per cent but it is poorly quantified. If the same cross-sections are used in satellite observations and ground-based observations, one source for non-consistency can be excluded from the comparison allowing a relative rather than absolute comparison, but this is not always the case. In addition, when the uncertainties related to ozone cross-sections and their temperature dependencies are well characterized, this effect can be included in the error budget of ozone observations. It may be possible that this also improves the retrieval itself.

Part I Gap description

Primary gap type:

Knowledge of uncertainty budget and calibration

Secondary gap type:

Parameter (missing auxiliary data etc.)

ECVs impacted:

Ozone

User category/Application area impacted:

- Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.)
- Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)

Non-satellite instrument techniques involved:

- UV/VIS zenith DOAS
- UV/VIS MAX-DOAS
- Pandora

Related gaps:

- G2.37 Poorly quantified uncertainties in spectroscopic information

This gap represents the top-level coordination and harmonisation activity required across the general spectroscopic measurement field, therefore G2.26 should be addressed in parallel with G2.37.

Detailed description:

The ozone absorption cross-section is one of the main systematic error sources in the remote sensing of atmospheric ozone using UV-visible spectroscopy techniques. The uncertainty in the cross-sections can be considered as a systematic error source, although the actual error depends on atmospheric temperature, and thus it can be considered as a pseudo-random (or structured random) error, as mentioned in the deliverable D4.3 'Uncertainty Budget' of the EC FP7 project NORS . Presently the uncertainty in total column ozone due to uncertainty in absorption cross-sections is assumed to be around one to a few per cent (WMO GAW report 218 , NORS_D4.3_UB.pdf). In general, when the uncertainties related to ozone cross-sections and their temperature dependencies are well characterized, this effect can be included in the error budget of ozone observations. It is also possible that by including the (correlated) uncertainty to the retrieval algorithm, this would improve the retrievals as well.

The recent WMO IGACO-O3/UV activity ACSO (Absorption Cross Sections of Ozone) performed a thorough evaluation of the existing cross-sections and their impact on ground-based and satellite ozone retrievals. In particular, cross-sections studied were Bass and Paur (published in 1985), Brion, Daumont Malicet (published in 1995) and Serdyuchenko et al. (2014). The outcome of the ACSO study was that the latest Serdyuchenko et al. cross-sections are recommended to be used for ground-based Brewer and Dobson instruments. However, these cross-sections were not recommended to be used for satellite retrievals due to a deficiency in the signal-to-noise ratio close to 300nm. From the perspective of satellite validation, it would be beneficial if the same cross-sections were used by both satellites and ground-based instruments such that at a minimum a relative comparison were possible. However, if different absorption cross-sections are used in the satellite validation, it is important to understand what type of differences they cause in the validation. Related to GAIA-CLIM, it is to be noted that neither Pandora nor any other DOAS or MAX-DOAS instruments were included in the ACSO study.

Operational space missions or space instruments impacted:

- Copernicus Sentinel 5P, 4/5
- MetOp
- Polar orbiters
- Geostationary satellites
- UV/VIS nadir
- Passive sensors

Validation aspects addressed:

- Geophysical product (Level 2 product)

- Time series and trends
- Calibration (relative, absolute)
- Spectroscopy

Gap status after GAIA-CLIM:

After GAIA-CLIM this gap will remain.

A literature study leading to a summary of the findings including a recommendation of how this should be applied with regard to DOAS, MAX-DOAS and Pandora instruments has been undertaken in GAIA-CLIM but this does not close the gap.

Part II Benefits to resolution and risks to non-resolution

Identified benefit	User category/Application area benefitted	Probability of benefit being realised	Impacts
Using the same cross-sections consistently with satellite and ground based instrumentation improves comparison by reducing the uncertainty in one critical factor.	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	More reliable ozone products. Improved validation by improving the data consistency (removing one source of discrepancy in the respective data analyses).
Understanding the uncertainties of the cross-sections improves the error characterization of the ground based instrument.	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	Medium	Improved error characterization of the ozone products
Understanding the uncertainties of the cross-sections may improve the retrieval results if correctly taken into account in the data processing (e.g. correlated errors).	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation	Medium	Potentially improved ozone products and their uncertainties.

	and improvement of ECV Climate Data Records)		
Identified risk	**User category/Application area benefitted**	**Probability of benefit being realised**	**Impacts**
Error characterization is missing one component	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	Medium	Incomplete error characterization causing potential decrease in data quality.

Part III Gap remedies

Gap remedies:

Remedy1: Improved understanding of the effects of differences in ozone cross-sections

Primary gap remedy type:

Research

Secondary gap remedy type:

Technical

Specify remedy proposal:

It is necessary to study in-depth what impact the differences in the ozone cross-sections recommended for Dobson and Brewer instruments and the ones used for satellite retrievals have on the retrieved ozone amount when applied within the DOAS data analysis technique. This would be best achieved via a simulation study using the operational Pandora retrieval algorithm with alternative cross-sections of ozone but should also be added to the list of follow-up studies for the CINDI-2 intercomparison exercise. However, preliminary information should also be obtained from a literature study in consultation with the Brewer and Dobson communities and some original quantitative analyses. The analysis may be expected to lead to recommendations for future processing of measurements to be taken up by those networks operating these instruments. The analysis may also require additional dedicated measurements at a small number of sites to support the characterisation.

Relevance:

Starting from the results achieved within the ACSO study, the study proposed here will help to understand the uncertainties caused by different sets of ozone cross-sections used within the data analysis and how this impacts on the overall measurement uncertainty.

Measurable outcome of success:

If the difference in the end product (total column ozone) is quantifiable with regard to which of the different ozone cross-sections have been used within the retrieval, then this can be applied to better compare the ozone data measured by satellites with ground-based data sets while both satellite and ground-based observations still use their preferred ozone cross-sections for the data analysis.

Expected viability for the outcome of success:

Medium

Scale of work:

- Single institution
- Consortium

Time bound to remedy:

Less than 3 years

Indicative cost estimate (investment):

Low cost (< 1 million)

Indicative cost estimate (exploitation):

No

Potential actors:

- EU H2020 funding
- Copernicus funding
- ESA, EUMETSAT or other space agency
- Academia, individual research institutes

References:

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G2.27 Lack of understanding of random uncertainties, air mass factor calculations, and vertical averaging kernels in the total ozone column retrieved by UV-visible spectroscopy

Gap abstract:

The uncertainties in the ozone slant columns retrieved with DOAS data analysis fitting procedures are predominantly caused by instrumental imperfections and by issues introduced within the analysis routines. Such uncertainties are often random and therefore can be estimated statistically from, e.g., the least-squares fit procedure. However, the fitting uncertainties derived from such analysis typically result in unrealistically small uncertainties and can lead to an underestimate by up to a factor of two. Further uncertainties are introduced during the calculation of air mass factors (AMFs) which are required to convert the measured ozone slant columns into vertical columns. The AMF uncertainties are dominated by errors in a priori profile shape effects with ozone and pressure/temperature a priori profiles being key input parameters for the AMF calculations. For further interpretation of the total column observations, averaging kernel information as part of the retrieval product plays an important role. However, currently vertical averaging kernels are only approximations of the real 3D averaging kernel and cannot fully account for the representativeness of the data.

Part I Gap description

Primary gap type:

Knowledge of uncertainty budget and calibration

ECVs impacted:

Ozone

User category/Application area impacted:

- Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.)
- Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)

Non-satellite instrument techniques involved:

- UV/VIS zenith DOAS
- UV/VIS MAXDOAS
- Pandora

Related gaps:

- G2.37 Poorly quantified uncertainties in spectroscopic information

This gap represents the top-level coordination and harmonisation activity required across the general spectroscopic measurement field, therefore G2.27 should be addressed in parallel with G2.37

Detailed description:

This gap addresses three of the major individual issues in our understanding of the analysis processing chain from the raw spectrum to the final total column ozone data product using the DOAS technique, and the interpretation of the actual final product.

The first aspect is the uncertainties in the ozone slant columns retrieved with the standard DOAS data analysis fitting procedures. They are to a large part caused by (1) instrumental imperfections such as detector noise, resolution change, etaloning (a fault that develops in thin charge-coupled devices when they behave as etalons) and other non-linearities of the detector, stray-light, and polarisation effects, as well as (2) by issues introduced within the analysis routine such as uncertainties in the Ring effect, unknown absorbers, and the wavelengths dependency of the AMF. Such uncertainties are mostly random in nature and therefore can be estimated statistically from the least-squares fit procedure. However, the fitting uncertainties derived from the least-squares analysis typically result in unrealistically small uncertainties and can lead to an underestimate of the measurement uncertainty by up to a factor of two. Results from intercomparison exercises (e.g. Van Roozendael et al., 1998, Vandaele et al., 2005, Roscoe et al., 2010) show that state-of-the-art instruments hardly ever agree to better than a few percent, even when standardised analysis procedures are used. This indicates that the actual accuracy in the ozone slant columns is at least to some degree limited by uncontrolled instrumental and/or analysis factors. And it leads to the question if something is not yet adequately addressed in the fitting procedures.

Further uncertainties are introduced during the calculation of air mass factors (AMFs) which are required to convert the measured ozone slant columns into vertical columns which means that the measured slant column density (SCD) is divided by the AMF to calculate the vertical column density (VCD) in molecules/cm2 which is then converted into Dobson Units. The NDACC UV-visible spectroscopy working group recommends the use of a generic look-up table of ozone AMFs which has been developed at BIRA-IASB (see NDACC UV-vis working group report) and accounts for the latitudinal and seasonal dependencies of the ozone vertical profiles. The NDACC recommendation is furthermore to average all retrieved vertical columns of ozone between 86° and 91° Solar Zenith Angle (SZA). The recommended approach is to apply a linear fit on vertical columns in the above SZA range and then derive the column value at the effective SZA (so far recommended to be 90° SZA). This range minimizes the measurement uncertainties arising during the fitting procedures and AMF calculation, and provides stratospheric ozone measurements with limited sensitivity to tropospheric ozone and clouds. Ozone and pressure/temperature *a priori* profiles are key input parameters for the AMF calculations, and AMF uncertainties for zenith-sky twilight ozone retrievals are dominated by uncertainties in a priori profile shape effects. Hendrick et al. (2011) found that the uncertainty in the calculated AMFs based on uncertainties in the ozone profiles is around 1%. However, there is a lack of an adequate database of tropospheric ozone in particular, and in regions where tropospheric or stratospheric ozone contents deviate from the climatological values, uncertainties of several percent can be introduced in total column ozone retrievals. Apart from uncertainties in the ozone a priori profiles, further sources of uncertainty are based on uncertainties in the aerosol and cloud information used. The typically small impact of clouds on zenith-sky ozone UV-vis measurements at twilight is due to the fact that the mean scattering layer is generally located at higher altitude than that of the clouds. However, AMFs calculated for cloudy conditions can be systematically larger than AMFs calculated for non-cloudy conditions.

The DOAS ozone total column retrieval is implicitly dependent on an a priori tracer profile. The radiative transfer calculation within the DOAS analysis accounts for the sensitivity of the measurement to tracer concentrations at all altitudes. These sensitivities are implicitly weighted with the assumed tracer profile to produce the retrieved column.

The averaging kernel is proportional to this measurement sensitivity profile, and provides the relation between the retrieved quantities and the true tracer profile. The kernel therefore provides important information needed for a quantitative analysis of the satellite data (Eskes and Boersma, 2003 and references therein). The averaging kernel concept is by now well established in remote sensing. Applications are for instance the retrieval of profiles of atmospheric quantities like temperature and tracers like ozone from satellite measurements. Retrieval groups are increasingly including the kernel information in the profile data products disseminated to users. The look-up tables for total column ozone averaging kernels, provided by the NDACC UV-vis working group, have been developed based on the approach described by Eskes and Boersma (2003), i.e. the averaging kernel of a layer i can be approximated by the ratio of the box airmass factor of this layer i and the total airmass factor calculated from an O_3 profile climatology. The availability of averaging kernel information as part of the total column retrieval product is important for the interpretation of the observations, and for applications like chemical data assimilation and detailed satellite validation studies. However, vertical averaging kernels (when provided based on a climatology) are only approximations of the real 3D averaging kernel of a retrieval and cannot fully account for the representativeness of the data.

Operational space missions or space instruments impacted:

- Copernicus Sentinel 4/5
- Meteosat Third Generation (MTG)
- MetOp
- Polar orbiters
- Geostationary satellites
- UV/VIS nadir

Validation aspects addressed:

- Geophysical product (Level 2 product)
- Time series and trends
- Spectroscopy

Gap status after GAIA-CLIM:

GAIA-CLIM has partly addressed this gap but it will not be closed within GAIA-CLIM.

An in-depth uncertainty analysis has been undertaken under GAIA-CLIM but closure requires its verification and implementation.

Part II Benefits to resolution and risks to non-resolution

Identified benefit	User category/Application area benefitted	Probability of benefit being realised	Impacts
If the source of the differences between fit	Operational services and service development (meteorological	High Medium	Improvement in overall data quality & more realistic uncertainty

uncertainty and expected uncertainty is better understood, this would lead to an improvement in the fit quality	services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)		partitioning between the components
Standardisation of AMFs will improve the overall uncertainty in the measured total O_3 columns retrieved from zenith sky UV-visible measurements	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High Medium	Will improve the overall accuracy of the measured total ozone column retrieved from zenith sky UV-visible measurements.
Improving the climatological databases of a priori ozone profiles will improve the accuracy of the RT model calculations of the respective AMFs	Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High Medium	Will improve the overall accuracy of the measured total ozone column retrieved from zenith sky UV-visible measurements.
Including 3D averaging kernels for zenith-sky UV-visible ozone measurements	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High Medium	Improvement in the agreement between the different data sets (different sites as well as satellite/ground-based). Better agreement between observations at the edge of the polar vortex where the spatial and temporal gradients of the ozone field can be very large.
Identified risk	**User category/Application area benefitted**	**Probability of benefit being realised**	**Impacts**
If a distinct difference remains between realistic uncertainty estimates and the uncertainty calculated by the fitting routines, this will lead to undue confidence in reported data values.	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.)	High Medium	Higher and poorly quantified uncertainty in data products (such as ozone) measured with the DOAS technique leading to reduced utility in applications.

	Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)		
AMFs used by different groups are not standardized.	Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High Medium	Ozone measurements provided by different groups are not homogenized and will likely show some unknown bias from site to site or group to group.
Including 3D averaging kernels for zenith-sky UV-visible ozone measurements	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High Medium	Improvement in the agreement between the different data sets (different sites as well as satellite/ground-based) & better agreement between observations at the edge of the polar vortex where the spatial and temporal gradients of the ozone field can be very large.

Part III Gap remedies

Gap remedies:

Remedy 1 – Improve our understanding of the discrepancy between the calculated fitting uncertainty and the more realistically estimated total random error.

Primary gap remedy type:

Research

Secondary gap remedy type:

Technical

Specify remedy proposal:

The proposed action is to improve our understanding of the discrepancy between the calculated fitting uncertainty and the more realistically estimated total random error. This needs to be done, firstly, by evaluating all literature studies and other documentation available on this topic and, secondly, by using the results from the MAX-DOAS intercomparison campaign at Cabauw, the Netherlands, in September 2016, to provide more state-of-the-art data

for further investigation specifically tailored to this issue. As part of GAIA-CLIM, we have developed a traceability chain for total column ozone measured by DOAS instruments and as part of this study we investigated, as a case study for two NDACC stations, the individual elements and their respective uncertainties leading up towards the DOAS fitting procedure and the uncertainties calculated within the fitting procedure. This is providing the first step for a quantitative investigation into the observed discrepancies which needs to be further extended e.g. with sensitivity studies of the uncertainties of the single components as well as an investigation of the potential of cancelling out of individual uncertainty components. The existing GAIA-CLIM work needs to be extended to be applicable across the full range of MAX-DOAS instrumentation in usage globally.

Relevance:

This remedy is specific for measurements using UV-visible spectroscopic measurement techniques and it will address the existing gap by providing a better understanding on what causes the discrepancy between the calculated fitting uncertainty and the more realistically estimated total random uncertainty.

Measurable outcome of success:

The success will be measured by how much we can improve our understanding of the difference between the individual uncertainty estimates versus the uncertainty provided by the data analysis fitting routines.

Expected viability for the outcome of success:

Medium

Scale of work:

- Single institution
- Consortium

Time bound to remedy:

Less than 3 years

Indicative cost estimate (investment):

Low cost (< 1 million)

Indicative cost estimate (exploitation):

No

Potential actors:

- EU H2020 funding
- Copernicus funding

- National funding agencies
- ESA, EUMETSAT or other space agency
- Academia, individual research institutes

Remedy 2 – Improvements to climatological databases of a priori ozone profiles for use in retrievals

Primary gap remedy type:

Research

Specify remedy proposal:

Improve climatological databases of a priori ozone profiles, with particular emphasis on tropospheric ozone are required to inform improved retrievals. It is necessary to test the quality/suitability of the databases of ozone profiles through a comparison with ozonesonde profiles at a selection of stations. Preferably this is to be done at the actual measurement site or station where also the UV-visible measurements are made. The vertically high resolved ozonesonde profiles can then be used to validate in particular the tropospheric part of the climatological ozone database. This would then specifically validate and improve the input parameters for the AMF calculation for that specific station. For NDACC stations, for example, which have both measurement techniques on site, this is a very feasible approach. Additionally, ozone profiles measured as part of ozonesonde networks, such as SHADOZ, provide this kind of validation for the currently used climatological database in a more global sense.

Relevance:

Improving the climatological databases of a priori ozone profiles will improve the accuracy of the a priori data used within the respective RT model to calculate the AMFs and hence to improve the overall accuracy of the measured total ozone column retrieved from zenith sky UV-visible measurements.

Measurable outcome of success:

If we can show that the updated and improved ozone database, when used as a priori for the ozone AMF calculations, leads to a smaller uncertainty in the calculation of ozone AMFs then we know that we have succeeded.

Expected viability for the outcome of success:

Medium

Scale of work:

- Single institution
- Consortium

Time bound to remedy:

Less than 3 years

Indicative cost estimate (investment):

Low cost (< 1 million)

Potential actors:

- EU H2020 funding
- Copernicus funding
- National funding agencies
- ESA, EUMETSAT or other space agency
- Academia, individual research institutes

Remedy 3 - Standardize AMF calculation methods and databases of a-priori information used in AMF calculations to improve the accuracy of the measured total column ozone

Primary gap remedy type:

Research

Specify remedy proposal:

Differences between AMFs can cause discernible discrepancies between the ozone data sets. For example, some NDACC UV-visible groups use their own individual DOAS settings and ozone AMFs calculated with different RTMs and sets of ozone, pressure and temperature profiles as input data, and with or without latitudinal and seasonal variations. The objective of the recommendations formulated by the NDACC UV-visible WG previously was thus to reduce these discrepancies through the use of standardized DOAS settings and ozone AMF look-up tables that account for the latitudinal and seasonal dependencies of the ozone vertical profile (see Hendrick et al., 2011).

The next step is to review, update and expand these existing tables further by initiating a targeted effort which also incorporates all relevant findings previously attained within projects such as NORS as well as investigations undertaken within GAIA-CLIM. Projects such as FRM4DOAS which are using centralised processing for the ozone data analysis also promote the use of more standardized AMF calculations and databases. With all this in mind, setting up a project to review and investigate the best routines and input variables for the AMF calculations, and to then recalculate and update the NDACC AMF LUTs to be used to homogenise the ozone total column data measured at different locations would be an efficient way forward.

Relevance:

Standardized AMFs will improve the overall accuracy of the measured total ozone column retrieved from zenith sky UV-visible measurements.

Measurable outcome of success:

Determine the difference between standardized AMFs and individually calculated ones and, in turn, the difference in the calculated vertical ozone columns. If the standardized AMF lead to smaller uncertainties in the total column ozone datasets we know that the remedy was successful.

Expected viability for the outcome of success:

Medium

Scale of work:

- Single institution
- Consortium

Time bound to remedy:

Less than 3 years

Indicative cost estimate (investment):

Low cost (< 1 million)

Potential actors:

- EU H2020 funding
- Copernicus funding
- National funding agencies
- ESA, EUMETSAT or other space agency
- Academia, individual research institutes

Remedy 4 – Evaluation of 3D averaging kernels for zenith-sky UV-visible ozone measurements

Primary gap remedy type:

Research

Secondary gap remedy type:

Technical

Specify remedy proposal:

An evaluation of 3D averaging kernels for zenith-sky UV-visible twilight measurements based on AMF look-up tables is needed and a comparison with averaging kernels derived using a direct coupling of the retrieval with the output of a chemistry-transport model, in which the a priori profile used in the AMF calculation is replaced by a more realistic model-derived time and space dependent profile. To tackle this issue further, one or two specific retrieval algorithms coupled with chemistry-transport model output need to be selected to run an in-depth comparison with the averaging kernels retrieved based on the AMF LUTs. An important focus is that the averaging kernel calculated based on the AMF LUTs are representative enough to provide the information expected to add additional value to the actual measurements.

Relevance:

Many research groups are not setup to run their retrieval code coupled with a chemistry-transport model and so it is essential to have a less computationally demanding approach which can then be used much more widely. Hence it is vital to understand how the uncertainties increase using the method based on the look-up tables and how representative the vertical averaging kernel climatology is of real measurement conditions.

Measurable outcome of success:

Including 3D averaging kernels for zenith-sky UV-visible ozone measurements in satellite and model validation studies should improve the agreement between the different data sets, especially for UV-visible stations located in winter/spring at the edge of the polar vortex where the spatial and temporal gradients of the ozone field can be very large.

Expected viability for the outcome of success:

Medium

Scale of work:

- Single institution
- Consortium

Time bound to remedy:

Less than 3 years

Indicative cost estimate (investment):

Low cost (< 1 million)

Indicative cost estimate (exploitation):

No

Potential actors:

- EU H2020 funding
- Copernicus funding
- National funding agencies
- ESA, EUMETSAT or other space agency
- Academia, individual research institutes

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G2.30 Metrologically incomplete uncertainty quantification for Pandora ozone measurements

Feedback

Gap abstract:

Pandora is a relatively new UV-VIS instrument for measuring total ozone and also ozone profiles in a similar way as MAX-DOAS instruments. So far only a few studies exist which describe measurement uncertainties or measurement validation. As a relatively inexpensive and automated instrument, there is a strong potential that a network of Pandora instruments could have a substantial role in the satellite validation in the future. A metrologically rigorous uncertainty quantification for the Pandora instrument is therefore needed.

Part I Gap description

Primary gap type:

Knowledge of uncertainty budget and calibration

Secondary gap type:

Governance (missing documentation, cooperation etc.)

ECVs impacted:

Ozone

Non-satellite instrument techniques involved:

Pandora

Related gaps:

- G2.31 Incomplete understanding of the different retrieval methods, information content, and random and systematic uncertainties of MAX-DOAS tropospheric ozone measurements

There are similarities in filling this gap and G2.31 is related to MAX-DOAS instruments even though there are no critical dependencies.

Detailed description:

Pandora is a relatively new UV-VIS instrument for measuring total ozone and also ozone profiles in a similar way as MAX-DOAS instruments. The instrument is relatively small, inexpensive and automatic. The number of Pandora instruments has been growing during recent years and therefore it is possible that a network of Pandoras could have stronger role in satellite validation in the future. For example, the European Space Agency has recently supported the development of Pandora network called Pandonia.

However, so far only a few studies exist which describe measurement uncertainties or measurement validation (see e.g. Herman et al. 2015, Tzortziou et al, 2012). This yields low confidence that the measurement uncertainties are currently either fully documented or rigorously quantified. For example, systematic uncertainty in Pandora direct-sun measurements are limited by temperature effects not corrected in current operational procedures. The neglect of temperature effects (related to the ozone spectroscopy in the Huggins bands) leads to seasonally dependent systematic biases and synoptic scale biases, of various amplitudes depending on the latitude of the site. This gap is partially addressed within GAIA-CLIM.

Operational space missions or space instruments impacted:

- Copernicus Sentinel 5P, 4/5
- MetOp
- MetOp-SG
- Polar orbiters
- Geostationary satellites
- UV/VIS nadir
- Passive sensors

Validation aspects addressed:

- Geophysical product (Level 2 product)
- Gridded product (Level 3)
- Assimilated product (Level 4)
- Time series and trends

Gap status after GAIA-CLIM:

After GAIA-CLIM this gap remains unaddressed.

A literature review has been initiated on the uncertainties related to total ozone retrievals using the Pandora instrument. Based on this and additional information obtained during the CINDI-2 campaign, an analysis of selected types of uncertainties is currently being completed. We expect, in particular, that the outcomes of the CINDI-2 campaign held in September 2016 will provide additional input for this gap. Several Pandora instruments as well as MAX-DOAS instruments have participated in the campaign. Exercises and studies performed during this campaign will provide the community with relevant datasets and information about how to proceed most effectively.

Part II Benefits to resolution and risks to non-resolution

Identified benefit	User category/Application area benefitted	Probability of benefit being realised	Impacts
Understanding of uncertainties related to Pandora instrument. In particular, understanding of systematic errors would be beneficial.	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Improved validation possibilities by using a relatively inexpensive and (quasi-)autonomous instrument.
Identified risk	**User category/Application area benefitted**	**Probability of benefit being realised**	**Impacts**
Potential systematic errors may limit satellite validation if not taken into account in the validation.	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	Medium	Potential source of systematic errors that are correlated in time and space.

Part III Gap remedies

Gap Remedies:

Remedy1: Instigate a reference quality measurement program for Pandora measurements

Primary gap remedy type:

Research

Secondary gap remedy type:

Technical

Specify remedy proposal:

A literature review undertaken in consultation with the Pandora community will provide a better quantification of the measurement uncertainties. This literature review should be supported by findings from the CINDI-2 campaign. Potentially, sensitivity studies to simulate the effects of various uncertainties in the retrieval setup are also needed to fully characterize the uncertainties of the ozone observations. A substantive analysis is required in consultation with experts in metrology to ensure a fully traceable uncertainty can be quantified. This may require modifications to instrument protocols down the line. Key facets of a traceable measurement are: Derivation of measurement equation and traceability diagrams, quantification of effect uncertainties, standardisation of measurement procedures and documentation of the methods deployed.

Within GAIA-CLIM, a detailed traceability chain has already been developed for total column ozone measurements made using UV-visible spectroscopic instruments and for this chain, each of the elements has been described in detail and the corresponding uncertainties have been quantified. Once this traceability chain together with the uncertainty details of the elements have been finalised, this information will be made available publicly and should provide a vital input towards the development of a metrologically rigorous uncertainty quantification for the Pandora instruments. Further work remains to have this processing adopted and the reference quality measurements provided on an operational basis to end-users.

Relevance:

Given that the Pandora instruments will form the backbone of a new measurement network (PANDONIA) run in close collaboration with NDACC, any better understanding of and reduction in the measurement uncertainties will contribute to the homogenisation of the ozone data products available within these networks.

Measurable outcome of success:

The aim is to reduce the total uncertainty of the final ozone data product and to understand the uncertainty budget and to quantify it in a metrological sense.

Expected viability for the outcome of success:

High

Scale of work:

Individually
Single institution

Time bound to remedy:

Less than 3 years

Indicative cost estimate (investment):

Low cost (< 1 million)

Indicative cost estimate (exploitation):

No

Potential actors:

- EU H2020 funding
- Copernicus funding
- National funding agencies
- ESA, EUMETSAT or other space agency

References:

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G2.31 Incomplete metrological understanding of the different retrieval methods, information content, and random and systematic uncertainties of MAX-DOAS tropospheric ozone measurements

Gap abstract:

Retrieving tropospheric ozone from passive remote sensing observations is difficult because almost 90% of the total column ozone resides in the stratosphere. Pioneering studies have demonstrated that information on tropospheric ozone can be extracted using the so-called MAX-DOAS (Multi-Axis Differential Optical Absorption Spectroscopy) technique. The information content of such measurements, however, remains to be thoroughly explored. Furthermore, within these studies, different experimental retrieval methods have been applied and more research is needed to better characterize the different possible approaches for tropospheric ozone retrieval. In addition to the lack of understanding of the information content and consensus on retrieval approaches, the lack of uncertainty characterization of tropospheric ozone measurements from MAX-DOAS instruments restrains the potential for the assessment of network capabilities and the usage of these data for satellite and model validation purpose.

Part I Gap description

Primary gap type:

Knowledge of uncertainty budget and calibration

Secondary gap type:

Vertical domain and/or vertical resolution
Technical (missing tools, formats etc.)
Parameter (missing auxiliary data etc.)

ECVs impacted:

Ozone

User category/Application area impacted:

- Operational services and service development (meteorological services, environmental services, Copernicus Climate Change Service (C3S) and Atmospheric Monitoring Service (CAMS), operational data assimilation development, etc.)

- International (collaborative) frameworks and bodies (SDGs, space agencies, EU institutions, WMO programmes/frameworks etc.)

Related gaps:

- G2.26 Poorly understood uncertainty in ozone cross-sections used in the spectral fit for DOAS, MAX-DOAS, and Pandora data analysis
- G2.27 Lack of understanding of random uncertainties, air mass factor calculations, and vertical averaging kernels in the total ozone column retrieved by UV-visible spectroscopy
- G2.30 Metrologically incomplete uncertainty quantification for Pandora ozone measurements

All these related gaps deal with the characterisation and improvement of the data quality of UV-visible measurements and, hence, should be considered at the same time or prior to the resolution of this gap.

Detailed description:

During the last decade, passive MAX-DOAS (Multi-Axis Differential Optical Absorption Spectroscopy) instruments have been deployed worldwide, focusing on the monitoring of air quality tropospheric trace gas species (NO_2, HCHO, SO_2, CHOCHO) but also halogens (BrO, IO) and aerosols (through oxygen dimer (O_4) measurements). Because they have similar spatial domains, MAX-DOAS is widely used to validate satellite nadir observations of pollutants like NO_2, HCHO, and SO_2 (see e.g. Hassinen et al. (2016) for the validation of the GOME-2 instruments on board of the METOP-A and B platforms). As for all UV-visible DOAS data products (see e.g. Platt and Stutz, 2008), the MAX-DOAS retrieval is based on a two-step approach: (1) a spectral inversion step using the differential optical absorption spectroscopy (DOAS) method and providing the slant column densities (SCD, which is the trace gas concentration integrated along the effective light path), and (2) a subsequent conversion step which ultimately provides the end products (tropospheric vertical columns and/or profiles).

Compared to other trace gases, tropospheric ozone retrievals are much more challenging since most of the ozone column (90%) is located in the stratosphere and therefore dominates the total ozone absorption, making the separation between the tropospheric and stratospheric ozone absorption signals difficult. Moreover, given the fact that for tropospheric ozone, the spectral fitting is usually done in the Huggins bands (i.e. 300-340 nm), the retrieval problem cannot be considered as linear as for other trace gases, because of the strong ozone absorption in this wavelength range. These difficulties explain why a limited effort has been made to date by the DOAS Community on this topic: so far only the exploratory studies of Liu et al. (2006) and Irie et al. (2011), both based on the Optimal Estimation Method (OEM; Rodgers et al., 2000), and of Gomez et al. (2014) have been reported in the literature.

In Liu et al. (2006), the atmosphere is modeled on an Umkehr-type grid with 22 layers from 0 to ~60 km, in steps of ~2.5 km for each of the bottom 20 layers and ~5 km for the top two layers. The total column ozone is also treated as one element of the measurement vector. The difference between the integrated total column from the ozone profile and the constrained total column estimated from zenith-sky or direct-sun observations is then minimized in the retrievals simultaneously with those between measured and simulated radiances at different elevation angles. The a priori ozone profile used in the retrievals and its standard deviations are extracted from the Total Ozone Mapping Spectrometer (TOMS) version-8 climatology. To extract more available information from the measurements, the *a priori* constraint is relaxed by increasing the original a priori standard deviations in the troposphere. A correlation length of 5 km is used to construct the a priori covariance matrix for the whole atmosphere. Tropospheric aerosols corresponding to a visibility of 50 km and background stratospheric aerosols from the LOWTRAN climatology are used. The temperature profile is taken from the US Standard Atmosphere.

In Irie et al. (2011), a simpler description of the troposphere is used and the state vector consists of VCD times a factor f_{clm} VCD is defined as the vertical column density (VCD) for altitudes below 5 km. The ozone number density is fixed to 5.8×10^{11} molecules cm^{-3} at 5 km based on the US Standard Atmosphere and the vertical profile shape is assumed to be linear between 0 and 5 km. Then, the vertical profile of ozone below 5 km is determined depending on the VCD: a smaller VCD tends to yield a linearly increasing profile with altitude while a larger VCD produces a

linearly decreasing profile. It is assumed that ozone concentrations are more variable in the Planetary Boundary Layer (PBL) than in the lower free troposphere, as the primary target of the Irie et al. (2006) study is to see variations in PBL concentrations. Above 5 km, the *a priori* profile has been set to the US Standard Atmosphere ozone profile. However, the profile above 5 km has been made multipliable by a factor, f_{clm}, in the retrieval in order to ensure a smooth matching between the profile parts below and above 5 km. For each 30-min interval, the *a priori* VCD value and the corresponding error are set to 20% and 100% of the maximum ozone differential slant column density (DSCD) values. The *a priori* f_{clm} (±error) is set to 1.0±1.0. Regarding the aerosols, a fixed AOD value (0.2) is assumed together with an exponentially decreasing with height profile shape.

In Gomez et al. (2014), a new approximation is proposed to estimate ozone mixing ratios from MAX-DOAS measurements at high-altitude sites. The proposed method uses O_4 slant column densities (SCDs) at horizontal and near-zenith geometries to estimate a station-level differential path. This modified geometrical approach (MGA) takes advantage of a very long horizontal path to retrieve ozone mixing ratios in the range of a few pptv (parts per thousand by volume). Moreover, measurements and retrieval approaches should be thoroughly characterized in terms of uncertainty budget and information content (vertical sensitivity, horizontal representativeness, dependency on measurement and solar geometries, and atmospheric visibility).

Although there have been these exploratory studies discussed above, there is still a clear need for a significant research effort to be undertaken by the DOAS community in order to (1) develop reference methods/algorithms and recommendations for the retrieval of tropospheric ozone vertical profiles and columns from MAX-DOAS measurements, and (2) operationally apply these algorithms to all existing MAX-DOAS stations.

In particular, the following specific issues have been identified:

1. Lack of understanding of the information content of MAX-DOAS tropospheric ozone measurements. Although the studies discussed above have demonstrated the feasibility of tropospheric ozone measurements from UV-visible absorption measurements in both the Huggins and Chappuis bands (see Liu et al., 2006; Irie et al., 2011; Gomez et al., 2014), the information content of such measurements remains to be thoroughly explored in terms of vertical sensitivity, dependency on measurement geometry (in particular the number of viewing angles being sampled), dependency on atmospheric visibility (i.e. aerosol content), solar geometry, horizontal representativeness, etc. This current lack of knowledge of the information content of MAX-DOAS tropospheric ozone measurements restrains the usage of this technique for large scale ozone monitoring and satellite and model validation. A better characterization of this information content will contribute to the development of robust retrieval methods (see also Remedy #1).
2. Better characterization of the different MAX-DOAS tropospheric ozone retrieval methods needed. So far the retrieval methods applied are experimental and are either based on Optimal Estimation (OE) schemes (Liu et al., 2006; Irie et al., 2011) or on more simple approaches such as the modified geometrical approximation used in Gomez et al. (2014) to infer free-tropospheric ozone concentration from a high-altitude site. More work is necessary to better characterize the different approaches. Such characterization will, in turn, also contribute to a better understanding of the information content corresponding the MAX-DOAS tropospheric ozone measurements (see bullet 1) above and Remedy #1 below).
3. Lack of in-depth understanding of random and systematic uncertainties of MAX-DOAS tropospheric ozone measurements. A better characterization of these uncertainties will contribute to a more in-depth knowledge of the information content of the corresponding MAX-DOAS tropospheric ozone measurements. As for other trace gases, the main uncertainties are related to the estimation of the effective photon light path, which is dependent on the aerosol content and optical properties. Moreover, in the case of ozone, the interference with the strong ozone absorption taking place higher up in the atmosphere is potentially a significant source of systematic bias and a comprehensive error budget of tropospheric ozone retrieval from MAX-DOAS measurements is lacking. The lack of uncertainty characterization of tropospheric ozone measurements from MAX-DOAS instruments restrains the potential for network capabilities assessment and the usage of these data for satellite and model validation purpose.

Operational space missions or space instruments impacted:

- Copernicus Sentinel 4/5
- Meteosat Second Generation (MSG)
- MetOp
- Geostationary satellites
- Infrared nadir
- UV/VIS nadir

Validation aspects addressed:

- Geophysical product (Level 2 product)
- Time series and trends

Gap status after GAIA-CLIM:

GAIA-CLIM has partly closed this gap.

This gap has been partly addressed by GAIA-CLIM, in particular through the work done by the CINDI-2 MAX-DOAS Tropospheric Ozone Working Group. But many aspects of the gap remain.

Part II Benefits to resolution and risks to non-resolution

Identified benefit	**User category/Application area benefitted**	**Probability of benefit being realised**	**Impacts**
A better characterisation of the information content of MAX-DOAS tropospheric ozone measurements and retrievals will produce highly-relevant correlative data sets for model and satellite tropospheric ozone validation studies.	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Copernicus research and operational tropospheric ozone data products better assessed and validated.
Highly-relevant (worldwide MAX-DOAS instruments deployment; measurement frequency: every 20 minutes during daytime) correlative data sets for model and satellite tropospheric ozone validation studies	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.)	High	Copernicus research and operational tropospheric ozone data products better assessed and validated.

	Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)		
A better characterisation of the uncertainty budget of MAX-DOAS tropospheric ozone measurements and retrievals will produce highly-relevant (worldwide MAX-DOAS instruments deployment; measurement frequency: every 20 minutes during daytime) correlative data	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Copernicus research and operational tropospheric ozone data products better assessed and validated.
Identified risk	**User category/Application area benefitted**	**Probability of benefit being realised**	**Impacts**
Sub-optimal validation of model and satellite tropospheric ozone data when using MAX-DOAS observations with corresponding information content not fully characterized or insufficiently understood and characterized uncertainty	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Potentially less confidence in satellite and model data due to the lack of highly relevant correlative tropospheric O_3 data sets

Part III Gap remedies

Gap remedies:

Remedy 1 Improved metrological understanding of potential for MAX-DOAS high-quality measurements and retrieval techniques of tropospheric ozone

Primary gap remedy type:

Research

Secondary gap remedy type:

Deployment

Specify remedy proposal:

More studies are needed to investigate the potential of the MAX-DOAS remote-sensing technique for tropospheric ozone measurements. In particular, the information content (vertical sensitivity, horizontal representativeness, dependency on measurement and solar geometries, and atmospheric visibility) and uncertainty budget of those measurements must be thoroughly characterized in different spectral ranges covering both Huggins and Chappuis ozone absorption bands and for a broad range of observation geometries and atmospheric conditions. Ideally, this should be conducted in a coordinated way, e.g. as part of an instrument intercomparison experiment such as the CINDI-2 intercomparison campaign which took place in Cabauw (The Netherlands) in September 2016. More in-depth studies are also needed to investigate and characterize the different possible methods for the retrieval of tropospheric ozone from MAX-DOAS observations. With most of the active MAX-DOAS research groups involved and the creation of a dedicated MAX-DOAS Tropospheric Ozone Working Group, this campaign provides an ideal framework for these tasks, and some of these tasks are already being addressed as part of the CINDI-2 campaign effort.

Hence the recommendation is:

To provide an in-depth characterisation of the different retrieval methods and their advantages and disadvantages for the retrieval of tropospheric ozone from MAX-DOAS measurements, and to select one of them for its operational application at all MAX-DOAS sites.

To provide the corresponding retrieval results to Copernicus and Space Agencies (ESA, EUMETSAT) for validation purpose.

Relevance:

A better characterisation of the information content and uncertainty budget of MAX-DOAS tropospheric ozone retrievals will improve the usability of MAX-DOAS observations for model and satellite validation studies, while an improved characterisation of the MAX-DOAS tropospheric ozone retrieval is fully aligned with the requirements of providing traceable and harmonized tropospheric ozone vertical columns and profiles for satellite and model validation.

Measurable outcome of success:

To provide MAX-DOAS tropospheric ozone retrieval results with improved information content characterization and uncertainty assessment to Copernicus and Space Agencies (ESA, EUMETSAT), and to estimate the impact of these improvements on the interpretation of model and satellite validation studies.

Expected viability for the outcome of success:

Medium

Scale of work:

- Single institution
- Consortium

Time bound to remedy:

Less than 3 years

Indicative cost estimate (investment):

Low cost (< 1 million)

Indicative cost estimate (exploitation):

No

Potential actors:

- Copernicus funding
- ESA, EUMETSAT or other space agency
- Academia, individual research institutes

References:

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G2.36 Lack of traceable uncertainties in MWR measurements and retrievals

Gap abstract:

Ground-based microwave radiometers (MWR) provide continuous and unattended retrievals of atmospheric temperature and humidity profiles, as well as of vertically-integrated total column water vapour (TCWV) and cloud liquid water (TCLW). Despite the significant scientific advancements allowed by MWR observations over the last forty years, current operational MWR retrievals are still lacking a traceable uncertainty estimate. The characterization of the total uncertainty budget for MWR retrievals requires quantification of the contributions from the instrument hardware (including absolute calibration) and the retrieval method (including the radiative transfer model). These contributions have been quantified in open literature, but they often refer to one particular instrument and/or environmental condition, and thus are not able to be generalized. A systematic approach that dynamically evaluates the total uncertainty budget of MWR (i.e. as function of instrument/environment conditions) at the network level is lacking. Initiatives for mitigating this gap are being undertaken in Europe as well as in the United States.

Part I Gap description

Primary gap type:

Knowledge of uncertainty budget and calibration

Secondary gap type:

- Uncertainty in relation to comparator measures
- Technical (missing tools, formats etc.)
- Governance (missing documentation, cooperation etc.)

ECVs impacted:

- Temperature
- Water vapour

User category/Application area Impacted:

- Operational services and service development (meteorological services, environmental services, Copernicus Climate Change Service (C3S) and Atmospheric Monitoring Service (CAMS), operational data assimilation development, etc.)
- International (collaborative) frameworks and bodies (SDGs, space agencies, EU institutions, WMO programmes/frameworks etc.)

Non-satellite instrument techniques involved:

Microwave Radiometer

Related gaps:

- G2.13 Missing microwave standards maintained by national/international measurement institutes
  G2.13 should be addressed with G2.36

Argument: The remedy of G2.13, i.e. the development of MW standards maintained at national/international measurement institutes and the availability of transfer standards, will set the basis for SI-traceability of MWR observations and retrievals. However, tools for evaluating the MWR total uncertainty budget can be developed independently of the solution of G2.13.

Detailed description:

The characterization of the total uncertainty budget for MWR retrievals requires quantification of contributions from the instrument hardware and the retrieval method. These contributions have been quantified in the open literature (e.g. Han and Westwater 2000; Hewison, 2006; Maschwitz et al., 2013; Stähli et al., 2013), but they often refer to one particular instrument and/or set of environmental conditions, and thus should not be generalized.

A proper uncertainty quantification for MWR retrievals shall result from the propagation of the uncertainty in calibration (transfer from raw voltages to the primary observable, the brightness temperature Tb) and the uncertainty in the retrieval method (transfer from Tb to atmospheric variables). As the uncertainty depends on the instrument and environmental conditions, the quantification shall be made dynamically, such that each measurement will be associated with one, generally different, uncertainty. The estimated uncertainty is thus time-and, for profiles, height-dependent. For a MWR network, the estimated uncertainty is also space-dependent, as it will depend on the instrument types deployed at various sites.

A systematic approach that dynamically evaluates the total uncertainty budget of MWR at the network level is lacking. In the following, the contributions to the total uncertainty are divided into four aspects: calibration and instrument characterization, retrieval method, radiative transfer and absorption model uncertainty, quality control.

<u>Calibration and instrument characterization</u>

Calibration and instrument characterization of MWR are to be performed regularly as they are time-dependent. Common procedures are applied by the operators to perform MWR calibration and instrument characterization. Currently, these procedures are usually provided by the manufacturers, and thus they are instrument-specific, or are based on user experience, and thus may be site-specific. Therefore, there is currently a lack of standardization in calibration procedures and uncertainty characterization. This in turn impacts negatively on the uniformity of products provided by a heterogeneous MWR network. This gap shall need to be addressed at both manufacturer and network levels.

<u>Retrieval method</u>

Different methods are currently applied for the retrieval of atmospheric variables from MWR observations. Different retrieval methods are adopted by different MWR manufacturers, operators, and users. Common retrieval methods include, but are not limited to, multivariate regression, neural networks and optimal estimation. This situation holds true for heterogeneous networks, such as the one currently establishing in Europe. The uncertainty of MWR retrievals depends partially on the used retrieval method. Documentation, versioning, and settings are usually not

accessible nor maintained. Information on retrieval uncertainty is often completely missing. The traceability of software documentation and versioning is also not guaranteed. This lack of coordination impacts negatively on the harmonization and spatio-temporal consistency of products from a heterogeneous MWR network. This gap shall need to be addressed at the network level.

Radiative transfer and absorption model uncertainty

Most common MWR retrieval methods are based on radiative transfer simulations through the atmospheric medium. Thus, uncertainties in modelling the absorption/emission of microwave (MW) radiation by atmospheric gases and hydrometeors affect all the retrieval methods based on simulated MW radiances. Only retrieval methods based on historical datasets of MWR observations and simultaneous atmospheric soundings are not affected by absorption model uncertainties. Currently, the information on MW absorption model uncertainties are dispersed and not easily accessible. Most operational MWR operate in the 20-60 GHz range, where relevant absorption comes from water vapour, oxygen, and liquid water. A variety of models are available which combine the absorption of water vapour, oxygen, and liquid water, as well as other minor contributions. Absorption model uncertainties are currently estimated from the output difference of different models, while a more rigorous estimate is lacking. An attempt to mitigate this gap is currently being carried out within GAIA-CLIM.

Quality control

Quality control (QC) procedures are fundamental for providing users with tools for judging and eventually screening MWR data and products. Most operational MWRs apply QC procedures that are developed by either the MWR manufacturer or by the operators based on their experience. There are different levels of QC procedures, going from sanity checks of the system electronics, to monitoring the presence of rain/dew on the instrument window, to radio frequency interference detection, to monitoring calibration against independent reference measurements (usually by radiosondes). The nature of the QC procedures varies, as these may be applicable to all instruments or conversely be instrument and/or site specific. Therefore, there is currently a lack of harmonization and automation of MWR QC procedures. This impacts on the quantity and quality of the data delivered, as poor QC may result in either delivery of faulty data, or screening out of good data. This gap shall need to be addressed at both manufacturer and network levels.

Operational space missions or space instruments impacted:

- Meteosat Third Generation (MTG)
- MetOp-SG
- Polar orbiters
- Geostationary satellites
- Microwave nadir
- Passive sensors
- GNSS-RO
- Other, please specify:
- Temperature and humidity sounders in general

Validation aspects addressed:

- Radiance (Level 1 product)
- Geophysical product (Level 2 product)
- Gridded product (Level 3)
- Assimilated product (Level 4)

- Time series and trends
- Calibration (relative, absolute)
- Spectroscopy

Gap status after GAIA-CLIM:

GAIA-CLIM has partly closed this gap.

Attempts to mitigate this gap are currently being carried out within and outside of GAIA-CLIM. Within GAIA-CLIM, a review of state-of-the-art MW absorption models and associated uncertainty has started (Cimini et al., 2017a). The absorption model uncertainties need to be propagated through radiative transfer and inverse operator to estimate the total uncertainties affecting the simulated brightness temperatures and the retrieval methods. A review paper shall collect the outcome of this analysis.
Outside of GAIA-CLIM, attempts to mitigate this gap are currently being carried out in the framework of the EU COST Action TOPROF, specifically by the Microwave Radiometer Working Group (WG3). WG3 is actively tackling the above challenges by interacting with manufacturers and users. WG3 produced a report on calibration best practices. New developments on calibration target design have been stimulated through the interactions with manufacturers. Network-suitable retrieval methods are currently under development within TOPROF WG3 (De Angelis et al. 2016; 2017). The role of GAIA-CLIM is to follow the developments at TOPROF and report to GAIA-CLIM as well as MWR users/manufacturers.

The present overarching MWR gap will be considered closed when procedures for MWR calibration and instrument characterization and a unified retrieval method will be performed uniformly across the network.

Part II Benefits to resolution and risks to non-resolution

Identified benefit	**User category/Application area benefitted**	**Probability of benefit being realised**	**Impacts**
Availability of best practices for MWR calibration and instrument characterization	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.)	High Medium	Best practices procedures will help operators in producing quality MWR observations and related uncertainty
Availability of a homogeneous and unified MWR retrieval method	Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	A network-wide common retrieval method will make documentation, versioning, and maintenance easier. It will guarantee spatio-temporal consistency of retrieval across the network
Full characterization of the uncertainty related to microwave absorption model	Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	The contribution to uncertainty due to microwave absorption model can be fully accounted in the uncertainty budget of MWR retrieved products

			and the associated time series and trends.
Availability of unified tools for automated MWR data quality control	Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High Medium	Trustable and unified tools for automated MWR data quality control will make MWR observations less user-dependent and thus more uniform across the network
Increased confidence in MWR retrieved products	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	The following will yield increased confidence and utilization of MWR observations in reanalyses and climate research: - Instrument- and site-independent procedures for MWR calibration and characterization - Understanding absorption model uncertainties - Network-wide consistent retrieval method, with sustained versioning and documentation - Trustable MWR data quality control
Identified risk	**User category/Application area benefitted**	**Probability of benefit being realised**	**Impacts**
Continued non-uniform practices for MWR calibration and error characterization	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.)	High	Higher probability of human error in MWR calibration and error characterization. Lack of network-harmonised MWR products which reduces their utility to applications requiring cross-network harmonised values such as satellite cal/val.
Lack of rigorous estimate for MW forward model uncertainty	Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Uncertainty of ground-based MWR retrievals lacks the contribution of the absorption model, which potentially affects time series and trend recognition
Quality of MWR products varying throughout a network	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	Lack of network-harmonised MWR products leading to challenges for applications that require a harmonised network of measurements such as satellite cal/val

Continued lack of unified tools for automated MWR data quality control	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)	High	MWR observations will continue to depend substantially on user experience. This can potentially introduce fake time/location differences. Quality uniform network products would be hampered.
Inspection by eye is recommended to detect suspicious data and faulty calibration	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.)	High	Additional personnel costs, prone to human error
Decreasing trust in MWR data quality	Operational services and service development (meteorological services, environmental services, Copernicus services C3S & CAMS, operational data assimilation development, etc.) International (collaboration) frameworks (SDGs, space agency, EU institutions, WMO programmes/frameworks etc.)	High	MWR users at operational services may not necessarily be able to develop their own QC procedures. Features caused by quality uncontrolled data may impact the trustiness and use of MWR systems. Lack of harmonization across the MWR network may negatively impact the trustiness of MWR systems.
Non-traceable MWR-based validation for satellite ECVs	All users and application areas will suffer from it.	High	No traceable validation for satellite boundary layer thermodynamical profiles

Part III Gap remedies

Gap remedies:

Remedy 1 Adoption of an international approach to implement recommendations for addressing existing gaps in MWR operational products for climate monitoring utilization

Primary gap remedy type:

- Technical
- TRL 5-7

Secondary gap remedy type:

- Deployment
- Research
- Education/Training
- Governance

Specify remedy proposal:

In order to close this overarching MWR gap, specific work plans should be developed to all the four aspects mentioned above: calibration and instrument characterization, retrieval method, radiative transfer and absorption model uncertainty, quality control. This may be best achieved via a collective set of actions which would be best achieved as a single project but could also be achieved via smaller distinct units of work as follows:

Calibration and instrument characterization

The currently available practices for MWR calibration and instrument characterization shall be reviewed. From these, the best practices should be defined and reported, and the documentation shall be made available to operators and users. Close collaboration with MWR manufacturers is desirable. The starting point is the outcome of the Microwave Radiometers Working Group (WG3) of the EU COST Action TOPROF, ended in October 2017. TOPROF WG3 produced a report on recommendations for operation and calibration of MWR within a network (Pospichal et al., 2016).

Retrieval method

The different types and flavours of retrieval methods currently exploited shall be reviewed and reported. A common retrieval method is recommended for MWR belonging to a network. The recommended retrieval method must produce explicitly and transparently the time-dependent estimated uncertainty of each atmospheric retrievals. A software package for a common retrieval method shall be developed and maintained. The starting point is the outcome of the TOPROF WG3 (Cimini et al. 2017b).

Radiative transfer and absorption model uncertainty

Modifications of absorption models are continuously proposed within the open literature based on laboratory data and MWR field observations. To estimate the total uncertainties affecting the MWR retrievals, the following activities are needed: (i) a review of the state-of-the-art and the associated uncertainty of MW absorption models; (ii) propagation of absorption model uncertainties through radiative transfer and inverse operator. Activities in this direction have started within GAIA-CLIM and shall eventually lead to a review paper (Cimini et al. 2017a).

Quality control

MWR quality control (QC) procedures shall be harmonized and automated to the maximum extent possible. A common network-wide data processing would be recommendable for the network products. Activities in this direction have started within TOPROF WG3, actively interacting with manufacturers for proposing ways for QC automation. Results of these activities shall be transferred as recommendations to users and manufacturers.

Activities contributing to the solution of the above issues have started within the COST action TOPROF and GAIA-CLIM. These two projects are ending in October 2017 and February 2018, respectively. Currently no plan is set for following up on these activities with research-oriented projects. The members of the TOPROF core group have submitted a proposal to the Policy and Finance Advisory Committee of EIG EUMETNET (grouping 31 European Meteorological Services) for including MWR into the next phase of their E-PROFILE project. If accepted, part of

the above tasks may be accomplished in that framework, specially those concerning calibration and instrument characterization, and quality control. The next phase of E-PROFILE is scheduled for 2019-2023.

Relevance:

Once the above issues are addressed, traceable MWR observations and retrievals will be available together with the estimate of the time-dependent uncertainty uniformly across the network. The remedies above will foster:

- The application of standardized calibration and uncertainty characterization procedures by MWR manufacturers and users;
- The use of a common network-suitable retrieval method. This will harmonise the MWR network products. Product harmonization leads also to more solid characterization of uncertainties;
- The consideration of MW forward model uncertainties in MWR retrievals, as quantifying the MW absorption model uncertainties will provide a common reference for MWR retrieval methods;
- The application of improved QC procedures by MWR manufacturers and users. Better QC leads to more solid characterization of MWR retrieval uncertainties, as it reduces the impact of suspicious data and faulty calibration.

Measurable outcome of success:

The measurable outcome of success for the above specific remedies are the following:

- The number of MWR sites, users, and manufacturers adopting the proposed calibration and uncertainty characterization procedures;
- The number of MWR users and manufacturers considering the rigorous estimates of MW forward model uncertainties in their MWR retrievals;
- The number of MWR sites (i.e. network nodes) providing retrievals and associated uncertainty produced with the recommended uniform retrieval method;
- The number of MWR sites, users, and manufacturers adopting the proposed QC procedures.

Expected viability for the outcome of success:

Medium

Scale of work:

Consortium

Time bound to remedy:

Less than 5 years

Indicative cost estimate (investment):

Medium cost (< 5 million)

Indicative cost estimate (exploitation):

Yes

Potential actors:

- EU H2020 funding
- Copernicus funding
- National Meteorological Services
- Academia, individual research institutes
- SMEs/industry

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G2.37 Need for more complete metrological characterisation of spectroscopic information

Gap abstract:

Molecular spectroscopy provides the primary link between radiance and atmospheric gas composition. Full knowledge of the spectroscopic properties of a measurement could, in theory, provide a route to formal traceability for that measurement. The exact nature of the influence of spectroscopic uncertainties on the derived ECV products will vary according to the spectral region being measured and the specific details of the measurement technique being employed – and a series of related gaps have been identified. However, there would be a clear benefit in a top-level spectroscopic coordination activity that identifies and disseminates common issues and solutions, including a harmonised process for dealing with spectroscopic uncertainties and establishing spectroscopic traceability.

Part I Gap description

Primary gap type:

Knowledge of uncertainty budget and calibration

Secondary gap type:

Governance (missing documentation, cooperation etc.)

ECVs impacted:

- Temperature
- Water vapour
- Ozone
- Carbon Dioxide
- Methane

User category/Application area impacted:

- Operational services and service development (meteorological services, environmental services, Copernicus Climate Change Service (C3S) and Atmospheric Monitoring Service (CAMS), operational data assimilation development, etc.)
- International (collaborative) frameworks and bodies (SDGs, space agencies, EU institutions, WMO programmes/frameworks etc.)
- Climate research (research groups working on development, validation and improvement of ECV Climate Data Records)

Non-satellite instrument techniques involved:

- Lidar
- Microwave Radiometer
- FTIR
- Brewer/Dobson
- UV/VIS zenith DOAS
- UV/VIS MAX-DOAS
- Pandora

Related gaps:

- G2.26 Poorly understood uncertainty in ozone cross-sections used in the spectral fit for DOAS, MAX-DOAS and Pandora data analysis
- G2.27 Lack of understanding of random uncertainties, Air Mass Factor calculations, and vertical averaging kernels in the total ozone column retrieved by UV-visible spectroscopy

This gap represents the top-level coordination and harmonisation activity required across the general spectroscopic measurement field. There are two gaps identified under this broad topic, G2.26 and G2.27 which address issues related to particular spectral regions and specific issues in individual measurement techniques. In both cases, this coordination activity should take place in parallel with the more specific gap assessments.

Detailed description:

Molecular spectroscopy provides the primary link between radiance and atmospheric gas composition, and is a primary component of the theory of radiative transfer through the atmosphere. The spectroscopic properties of a gas are constant and therefore, if they are robustly characterised and all of the external and instrumental influence factors on a spectroscopic measurement method are assessed, then formal traceability could, in theory, be realised for any measurement using that method.

In addition to the spectroscopic issues relating to those techniques that directly use spectroscopic measurement methods to derive information on ECVs, spectroscopic parameters are also an integral part of radiative transfer (RT) codes. RT codes constitute the core of radiometric physical retrievals, such as optimal estimation methods. In addition, any data intercomparison/validation method that includes the use of RT codes will also be influenced by spectroscopic uncertainties. Such uncertainties will contribute to the overall uncertainty of the data intercomparison, and could be the source of, potentially unexpected, correlation between the different data sources.

The exact nature of the influence of spectroscopic uncertainties on the derived ECV products will vary according to the spectral region being measured and the specific details of the measurement technique being employed – and a series of related gaps have been identified that give examples of this. However, there would be a clear benefit in a top-level spectroscopic coordination activity that took an overview of the more detailed technical developments; identified and disseminated common issues and solutions; and potentially developed a harmonised process for dealing with spectroscopic uncertainties and establishing spectroscopic traceability. This final goal of formal traceability based purely on the spectroscopic assessment of the measurement is a very challenging one that is unlikely to be resolved in the short term. However intermediate steps to improve the knowledge of spectroscopic uncertainties and their impact on measurement methods and intercomparison results, will have immediate impact which will be enhanced through an overall spectroscopic coordination activity.

Historically, other sources of uncertainty have tended to be much larger than spectroscopic uncertainties such that spectroscopic uncertainty has tended to be seen as an ignorable effect. As satellite and non-satellite instrumentation become more stable and better characterised and understanding of collocation effects improves it

is increasingly the case that spectroscopic uncertainties become important or even the limiting factor in the comparison, particularly as they are a potential source of long term correlation within individual measurement methods but also in comparisons between methods. It is thus increasingly important that spectroscopic uncertainties be considered afresh and better quantified.

Operational space missions or space instruments impacted:

Independent of specific space mission or space instruments.

This gap relates to all space instruments that rely on knowledge of spectroscopic parameters in their measurement procedure or could use a sub-orbital spectroscopic-based technique as a validation tool.

Validation aspects addressed:

- Radiance (Level 1 product)
- Geophysical product (Level 2 product)
- Spectroscopy

Gap status after GAIA-CLIM:

After GAIA-CLIM this gap will remain.

Part II Benefits to resolution and risks to non-resolution

Identified benefit	**User category/Application area benefitted**	**Probability of benefit being realised**	**Impacts**
A robust and consistent approach to the handling of uncertainties and traceability in spectroscopic measurements would significantly extend the availability of reference quality data across a wide range of techniques and ECVs.	All users and application areas will benefit from it	Medium	The provision of a formalised route to spectroscopic traceability would enable reference quality data to be realised in an efficient and consistent manner at any location. The contribution to uncertainty due to spectroscopic parameters can be fully accounted in the uncertainty budget of retrieved products and the associated time series and trends.
An improved understanding of the common issues in spectroscopic measurements would identify sources of correlated uncertainties between different measurement and modelling techniques	All users and application areas will benefit from it	High	Improved quality and understanding of the intercomparison between sub-orbital and satellite based measurements, and between measured and modelled atmospheric distributions.

			Understanding the spectroscopic uncertainties will yield increased confidence and utilization of observations in reanalyses and climate research.
Identified risk	**User category/Application area benefitted**	**Probability of benefit being realised**	**Impacts**
If a coordinated activity is not carried out then the situation will remain as a series of separate activities linked to individual techniques / instruments.	All users and application areas will suffer from it.	High	ECV retrieval uncertainty lacks a coordinated contribution of RT models, which may potentially affect time series and trend recognition. Intercomparison / validation activities remain inefficient with none of the synergistic benefits that a coordinated spectroscopic assessment could bring.
The potential effects of correlated uncertainties in the comparison of results from different techniques due to spectroscopic issues are not identified.	All users and application areas will suffer from it.	High	A key element in assessing the comparability and/or consistency of different measurements is not properly addressed, potentially undermining validation studies.

Part III Gap remedies

Gap remedies:

Remedy 1 Establish traceability of spectroscopic properties of Essential Climate Variables

Primary gap remedy type:

Research

Secondary gap remedy type:

Education/Training
Governance

Specify remedy proposal:

Establishment of a top-level cooperation and networking activity to coordinate and review spectroscopic uncertainty activities across the range of spectral regions and measurement techniques, with the long-term goal of developing harmonised processes to establish spectroscopic traceability in ECV determination. This may be achieved either by a large-scale coordinated project or piecemeal for specific cases. A large-scale coordinated project approach would benefit from synergies and commonality of approaches and may be preferred. Experts in laboratory and theoretical spectroscopy, metrology and the instruments would be required, and would need to link to the exiting collaborative activities involved in the development of spectroscopic reference databases such as HITRAN and GEISA. A key aspect of this work will be the introduction of metrological traceability in the determination of new spectroscopic data, covering both the target gas concentrations and path lengths being measured but also the ancillary parameters such as temperature, pressure and matrix gas composition that are crucial in derivation of spectroscopic model parameters and their uncertainties. The top level project should include a focus on the development of common procedures and robust methods that could be deployed across the wider spectroscopic community, to ensure consistency and comparability amongst data providers in the generation of the spectroscopic parameters, and understanding amongst data users in the application of the parameters and related uncertainties.

Relevance:

The proposed coordination activity is required to ensure a harmonised approach to addressing specific gaps in spectroscopic knowledge. This will lead to the efficient development of an improved understanding of spectroscopic uncertainties and a unified methodology in establishing traceability in spectroscopic measurements.

Measurable outcome of success:

Successful outcome of the activity will be demonstrated in the short term through transfer of knowledge from one area of spectroscopic research to another, and through the development of common processes and procedures. An additional measure of success would be the implementation of the estimated uncertainties in the retrieval methods exploited by the satellite and ground-based user community.

Expected viability for the outcome of success:

Medium

Scale of work:

Programmatic multi-year, multi-institution activity

Time bound to remedy:

More than 10 years

Indicative cost estimate (investment):

Medium cost (< 5 million)

Indicative cost estimate (exploitation):

Yes

Potential actors:

Other: European funding mechanisms such as COST or EMPIR.