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Gap Analysis for Integrated Atmospheric ECV Climate Monitoring:

Update for GAIA-CLIM Gaps Assessment and Impacts Document from WP3

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Authors	T. Verhoelst (BIRA-IASB), J.-C. Lambert (BIRA-IASB), D. Butterfield (NPL), T. Gardiner (NPL), R. Kivi (FMI-ARC), P. Kolmonen (FMI), G. de Leeuw (FMI), F. Madonna (CNR), L. Mona (CNR), A. Fassò (UniBergamo), K. Rannat (TUT)
Editors	T. Verhoelst (BIRA-IASB), J.-C. Lambert (BIRA-IASB)
Reviewers	Peter Thorne (NUIM), Corinne Voces (NUIM), Richard Davy (NERSC)
Contacts	Tijl.Verhoelst@aeronomie.be
URL	http://www.gaia-clim.eu

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Document history

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0.2	Tijl Verhoelst, Jean-Christopher Lambert	20/06/16	Previously identified gaps included and made SMART; Summary written.
1.0	All document authors and reviewers.	30/06/16	Additions and feedback from WP3 partners and WP leads included. Reviewed by project PI and management.

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Executive Summary

This deliverable constitutes further input from WP3 (Comparison error budget closure – Quantifying metrology related uncertainties of data comparisons) to the drafting of the living Gaps Assessment and Impacts Document (GAID) of Task 6.2 (WP6), led by KNMI. The purpose of the GAID is to collate and document gaps directly relevant to the aims of the GAIA-CLIM project. The GAIA-CLIM project is concerned with increasing the utility, use and value of non-satellite observations to characterise satellite observations. Further project details are available at www.gaia-clim.eu.

This deliverable refers to the second official release of the GAID (D6.4) and builds upon the gaps identified therein. In addition, it arises new gaps that have been identified in relation to the Work Package activities.

WP 3 deals with the additional errors and uncertainties that arise when measurements with different sampling and smoothing properties are compared in an inhomogeneous and variable atmosphere. Quantifying these errors requires an assessment of the natural variability, the full spatio-temporal sensitivity of the measurements, and of the adopted co-location criteria.

This deliverable further expands upon the gaps identified in the initial work package input, relevant gaps sourced externally, and new gaps that have been identified by participants. The gaps discussed herein are exclusively those related to the WP aims and remit (see prior paragraph). A key focus of the current iteration is to make the gaps and their remedies more SMART (Specific, Measurable, Actionable, Relevant and Timebound) with realistic cost estimates and assessments of the risk / cost of leaving the gap unremedied. In year 3 the GAID shall inform the development of a list of prioritised recommendations and this shift in emphasis is expected to help inform such an exercise.

1. Document rationale and broader context

The purpose of this document is to provide input to the Gaps Assessment and Impacts Document (GAID) of the GAIA-CLIM project arising from WP3. This WP is concerned with improving our quantification of the irreducible uncertainties that arise from inevitable non-coincidence of satellite and non-satellite measurements. The measurements may occur at different times or locations or they may be sensitive to different volumes. Because the atmosphere is often inhomogeneous and variable on the spatial and temporal scales of the co-location, any mismatch will lead to a difference that arises from changes in the atmospheric state. These differences must be accounted for in any meaningful comparison between the satellite and non-satellite measurements if reliable inferences are to be made. More specifically, the work package aims to:

- Characterise the uncertainties arising for individual measurement systems (Task 3.1, targeting Gap G3.04)

- Characterise the uncertainties arising for data comparisons (Task 3.2, targeting Gaps G3.02 and G3.06).

- Develop software tools to enable the integration of WP3 developments and results in the forthcoming “Virtual Observatory” (WP5, Task 3.3, targeting Gaps G3.02, G3.04, G3.06 and to some extent G3.03).

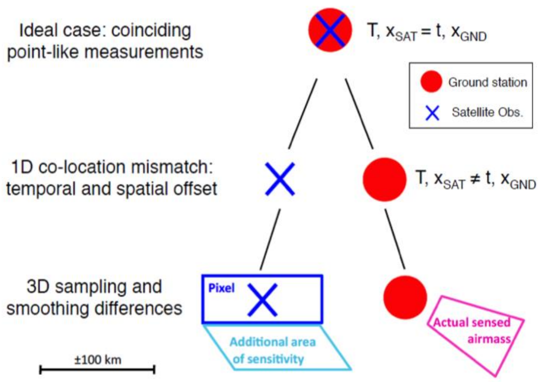

Figure 1: Conceptual visualisation of the metrology of a satellite-ground measurement comparison, from Verhoelst et al., 2015.

Results achieved so far within this work package include the writing and delivery (D3.2) of a technical note detailing generic metrology aspects of atmospheric composition measurements and their intercomparisons. This TN will serve as a technical background and guidance document to several future WP3 deliverables, such as D3.4, the report on measurement mismatch studies, D3.5, the tools to be implemented in the ‘Virtual Observatory’, and D3.6, the library of smoothing and sampling error estimates. Also, a detailed case study was elaborated, dealing with total ozone comparisons, and addressing in particular the gaps G3.04 and G3.06, and exploring briefly G3.02. This work was published by Verhoelst et al. (AMT, v.8, 2015). Ongoing work targets the same gaps, focussing also on other ECVs targeted by GAIA-CLIM, in particular temperature, humidity, and aerosol load. Besides the OSSE approach followed in the above-mentioned paper, also other approaches, such as the heteroskedastic statistical model of Fassò et al. (AMT, V.7, 2014), are followed.

To a large extent, this work is exploratory and it is far outside the scope of GAIA-CLIM to close all the gaps documented hereafter. The aim is rather to raise awareness of these co-location mismatch issues and to provide recipes, methods and recommendations on how future users of non-satellite measurements can both estimate and take into account these additional uncertainties, in particular in the context of satellite data validation. This aim is also pursued through participation in the International Space Science Institute (ISSI) team "EO validation across scales", lead by dr. A. Löw (University of Munich, Germany) and running for 15 months from 1/2016, including 3 meetings at ISSI, Bern. This team brings together different EO communities (CEOS-LPV, SST, LST, hydrology, atmosphere) to discuss validation strategies, with a particular focus on the point-to-area problem, which is closely related to WP3 within GAIA-CLIM.

The GAID has now gone through 2 iterations. The first iteration was based upon a combination of the user survey and individual inputs from this and the four remaining underlying Work Packages. The second iteration built upon this by incorporating feedback from the first user workshop and additional informal input delivered from this and other Work Packages. The third version shall build upon the second by considering input arising from this current set of deliverables. That version shall be discussed at the second user workshop to be held in Brussels in November 2016 and the input received shall lead to a further iteration, which shall form the initial basis for a set of prioritised recommendations arising from Task 6.3.

Feedback from the science advisory panel, the first General Assembly, and the review pointed collectively to the need to evolve the GAID to go beyond characterising the gap to considering in more detail implications, potential SMART remedies, costs, and the benefits of resolving them. This then shall help allow external and internal users to more fully explore and appreciate the gaps identified prior to work by Task 6.3 to collate a set of prioritised recommendations.

2. Summary of gaps from GAID v2 relevant to the current WP

The gaps identified in GAID that shall be considered in further detail in Section 4 are summarised below. This is a direct subset of relevant entries from Table 2.2 of the version 2 release of the GAID. These gaps arose from either the initial Deliverable from this WP (D3.1) or from subsequent external input. All gaps are assigned an owner within GAIA-CLIM, even if they arose from an external source.

Gap Identifier	Gap Type	ECV(s)	Gap Short Description	Trace
G3.01	Comparator unc.	H_2O, O_3, T, CO_2, CH_4, aerosols	Incomplete knowledge of spatiotemporal atmospheric variability at the scale of the inter-comparisons	D3.1 (incl. Annex 1, 2 and 3)
G3.02	Comparator unc.	H_2O, O_3, T, CO_2, CH_4, aerosols	Limited quantification of the impact of different co-location criteria on comparison results	D3.1 (incl. Annex 1, 2 and 3)
G3.03	Comparator unc.	H_2O, O_3, T, CO_2, CH_4, aerosols	Missing generic and specific standards for co-location criteria in validation work	D3.1 (incl. Annex 1, 2 and 3)
G3.04	Comparator unc.	H_2O, O_3, T, CO_2, CH_4, aerosols	Limited characterization of the multi-dimensional (spatiotemporal) smoothing and sampling properties of atmospheric remote sensing systems, and of the resulting uncertainties	D3.1 (incl. Annex 1, 2 and 3)
G3.05	Comparator unc.	H_2O, O_3, T, CO_2, CH_4, aerosols	Representativeness uncertainty assessment missing for higher-level data based on averaging of individual measurements	D3.1 (incl. Annex 1, 2 and 3)
G3.06	Comparator unc.	H_2O, O_3, T, CO_2, CH_4, aerosols	Missing comparison error budget decomposition including errors due to sampling and smoothing differences	D3.1 (incl. Annex 1, 2 and 3)

3. New gaps identified by WP participants to date

Subsequent to the first official input to the GAID (D3.1), substantial work has been undertaken upon the Work Package in the following respects:

- To describe -and raise awareness of- generic metrology aspects of an atmospheric composition measurement and of a data comparison,
- To quantify the errors and uncertainties to be taken into account on top of the measurement uncertainties, due to the multi-dimensional smoothing properties of ground-based and satellite measurements, for total ozone columns, aerosol load, temperature and humidity,
- To quantify the errors and uncertainties in data comparisons between satellite and non-satellite instruments resulting from imperfect co-location,
- To explore the impact of different co-location criteria on the significance of mismatch uncertainties in the total uncertainty budget.
- To explore solutions for integration of WP3 results into the VO.

These activities, in addition to advancing the aims of the GAIA-CLIM project, have given cause to reflect further on potential gaps in our collective knowledge and capabilities. This has not led to any additional gaps being identified at this time.

4. Detailed update on traces for the gaps arising from this Work Package for inclusion in the GAID

Within this section gaps that were detailed in Sections 2 and 3 are expanded to give a full trace of our current understanding of the gap, its impacts and its potential remedies. For those gaps identified in Section 2 we take as the starting point the corresponding text arising from the GAID (v2, Section 3) text and / or the initial deliverable text (D3.1) as we deem most appropriate. This is then expanded upon here in an attempt to better delineate the gap, its impacts, its potential remedies (including indicative costs and timelines) and the scientific impact of (non-)resolution. Gaps are ordered numerically and each given a specific subsection.

G3.01 Incomplete knowledge of spatiotemporal atmospheric variability at the scale of the measurements and their co-location

Gap detailed description

Spatiotemporal variability of the atmosphere at the scale of the airmass being measured or - in the case of a measurement intercomparison - at the scale of the co-location, leads to additional uncertainties, not accounted for by the uncertainty budget reported with an individual measurement. To quantify these additional uncertainties (cfr. gaps G3.04 and G3.06), or to ensure that they remain negligible through the use of appropriate co-location criteria (cfr. G3.03), a prerequisite is a proper understanding of atmospheric variability of the targeted ECV on those scales.

While scales above approx. 100km/1h are relatively well captured for several GAIA-CLIM target ECVs in model or satellite gridded data (e.g. Verhoelst et al., 2015, for total ozone), information on smaller scales is most often restricted to results from dedicated campaigns or specific case studies, e.g. Sparling et al. (2006) for ozone, Hewison (2013) for meteorological variables, and Pappalardo et al. (2010) for aerosols. Due to the exploratory nature of these studies, neither global nor complete vertical coverage is achieved. For instance, information on small-scale variability in the ozone field is limited to altitudes and regions probed with dedicated aircraft campaigns. The validation of satellite data records with pseudo global networks of ground-based reference instruments on the other hand requires an appropriate quantification of atmospheric variability in very diverse conditions, covering all latitudes, altitudes, dynamical conditions, degrees of pollution etc..

This gap therefore concerns the need for a better, more comprehensive, quantification of the spatiotemporal variability of the ECVs targeted by GAIA-CLIM. Note that this gap is also closely related to WP4 gap G4.06, which deals with the impact of natural variability on measurement-model comparisons, and with WP1 gap G1.07, dealing with the assessment of gaps in the existing networks.

Activities within GAIA-CLIM related to this gap

Resolving this gap is in general beyond the scope of the work planned within GAIA-CLIM. Nevertheless, some specific case studies in T1.4 (D1.9) targeting T, q, and aerosol load, and using measurements from polar orbiting sensors such as IASI and MODIS, will allow further insight and reveal in more detail to what extent this gap is a major hurdle in validation studies of these ECVs. These case studies can be considered to belong to the remedies based on (satellite) measurements (as detailed below).

Gap remedy(s)

Several approaches can aid in reducing and mitigating this gap. These can be either model or measurement based.

Remedy #1

Specific remedy proposed

High-resolution modelling studies at the global scale, resulting in comprehensive data sets of atmospheric fields.

Measurable outcome of success

The quality of the model output at its finest resolution can be estimated by comparison with high-resolution measurement data sets, preferably those with limited horizontal, vertical, and temporal smoothing effects, e.g. from balloon-borne sondes. Ideally, an agreement is found within the combined model and measurement uncertainty, and the model uncertainty itself is below that of the measurement (to maximize Relevance, see below).

Achievable outcomes

Improved spatio-temporal resolution in atmosphere models is a much broader scientific goal, with great computational and theoretical (e.g. convection and turbulence treatment) challenges. As such, this remedy probably requires a level of effort and resources beyond what can be driven by the need for satellite data validation. The technological/ organizational viability is therefore considered medium and the cost estimate high.

Relevance

If successful, this remedy would largely close the gap, and it would facilitate remedies for most other gaps identified here through the use of OSSEs (Observing System Simulation Experiments) based on these model fields.

Timebound

The development and computation of higher resolution (re-)analysis data sets at the major meteorological centres (e.g. ECMWF) typically requires several years of sustained effort.

Remedy #2

Specific remedy proposed

Statistical analysis of existing and future satellite and non-satellite high-resolution data sets, which allows to separate the contribution of atmospheric variability from the total uncertainty budget of a data comparison, e.g. using so-called ‘structure functions’ or heteroskedastic functional regression. Within the geographical and temporal coverage of the data set, these methods produce an estimate of the variability (or auto-correlation) of the field. Note that, as for Remedy #1, the scientific interest for higher resolution in the data sets is much broader than only the validation needs, e.g. for the identification of emission sources in an urban environment.

Measurable outcome of success

Publications describing for the different ECVs and various atmospheric regimes, locations and altitude ranges the atmospheric variability at scales ranging from those of in-situ measurements (e.g. 10s of meters for balloon sonde measurements) to that of a satellite pixel (several 10s to 100s of kilometres). These can be based either on exisiting data sets, or represent an exploitation of newly designed campaigns and missions.

Achievable outcomes

The technological and organizational effort required to make step changes in the spatiotemporal resolution of the observational data sets is in general very large, and comes with a large financial cost (more than 5 M euro), in particular if global coverage is aimed for. Hence, such developments need a much larger user base and the use proposed here should be considered secondary to the scientific objectives of such new missions. Nevertheless, smaller dedicated campaigns with for instance aircraft or Unmanned Aerial Vehicles (UAVs) can offer great insight at particularly interesting sites, and this at medium cost (between 1 and 5 M euro).

Relevance

This remedy directly addresses the gap, as already illustrated for instance with aircraft data for ozone by Sparling et al. (2006).

Timebound

The statistical analysis itself requires only a moderate amount of time (of the order of several months), but the design of dedicated field campaigns (up to a few years) or new satellite missions takes much longer.

Gap risks to non-resolution

Identified future risk / impact	**Probability of occurrence if gap not remedied**	**Downstream impacts on ability to deliver high quality services to science / industry / society**
Unknown impact of co-location mismatch on comparisons performed for validation purposes.	Very high	Interpretation of satellite data validation results severely hampered. This impacts negatively the reliability of the data sets, the reported uncertainties, and the products and services derived from these.

G3.02 Limited quantification of the impact of different co-location criteria on comparison results

Gap detailed description

Co-location criteria should represent an optimal compromise between the obtained number of co-located measurements (as large as possible to have robust statistical results) and the impact of natural variability on the comparisons (as low as possible to allow a confrontation between measured differences and reported measurement uncertainties). Hitherto, only a limited set of ground-based satellite validation studies explored the impact of the adopted co-location criteria on the comparison results (e.g. Wunch et al., 2011, and Dils et al., 2014, for CO_2, Verhoelst et al., 2015, for O_3, Pappalardo et al., 2010, for aerosols, and Van Malderen et al. 2014, for integrated water vapour). Still, atmospheric variability is often assumed –or even known- to impact the comparisons (e.g. De Maziere et al. 2008), but without detailed testing of several co-location criteria (or by extensive model-based simulations), this impact is hard to quantify. Besides the need for dedicated studies, from which clear recommendations could be formulated (cfr. gap G3.03), this gap also concerns the “community practices” regarding validation approaches, which often rely on a set of default (historical) co-location criteria, which are not necessarily fit-for-purpose for the accuracy and spatiotemporal sampling properties of current measurement systems.

Activities within GAIA-CLIM related to this gap

Two activities within GAIA-CLIM target this gap to some extent:

- Within task T3.2 in WP3, data intercomparison studies focussing on a closure of the comparison uncertainty budget include an exploration of different co-location criteria, see for instance the results on total ozone columns already published by Verhoelst et al. (2015, their Fig. 11).
- The Virtual Observatory developed in WP5 will offer the user the possibility to adjust co-location criteria and to visualize the resulting impact on the comparison results.

Gap remedy(s)

Remedy #1

Specific remedy proposed

Dedicated studies exploring in detail the advantages and disadvantages of several co-location methods and criteria. Dedicated working groups or activities could/should be set up within the framework of the ground-based observing networks, as already initiated for meteorological variables at a GRUAN-GSICS-GNSSRO WIGOS workshop on Upper-Air Observing System Integration and Application, hosted by WMO in Geneva in May 2014[1].

Measurable outcome of success

A peer-reviewed publication or a widely distributed technical note on the subject.

Achievable outcomes

The technical and organizational requirements for such studies are low, and so is the estimated cost, which is mostly to cover the salaries of the researchers involved.

Relevance

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[1] http://www.wmo.int/pages/prog/www/WIGOS-WIS/reports/3G-WIGOS-WS2014.pdf,

In view of the increasingly operational nature of satellite data validation using non-satellite data for the ECVs targeted within GAIA-CLIM (e.g. within the Copernicus context), such studies would be of high relevance, as they could support the definition of current and future validation protocols (cfr. also gap G3.03).

Timebound

This remedy should not require more than a year's FTE per ECV. Note that some additional effort will be required to re-address this gap when both the satellite and ground-based observing systems undergo step changes in their performance, e.g. for the upcoming geo-stationary platforms with much higher temporal sampling.

Gap risks to non-resolution

Identified future risk / impact	**Probability of occurrence if gap not remedied**	**Downstream impacts on ability to deliver high quality services to science / industry / society**
Poor feedback on data quality (in particular on the reported uncertainties) from validation studies due to unknown/unquantified influence of atmospheric variability.	Very high	Interpretation of satellite data validation results severely hampered. This impacts negatively the reliability of the data sets, the reported uncertainties, and the products and services derived from these.

G3.03 Missing generic and specific standards for co-location criteria in validation work

Gap detailed description

Different validation exercises on the same ECV/instrument combinations are often performed using different (sub-optimal) co-location criteria, ranging for instance from fixed maxima imposed on spatial and temporal distance (e.g. Ohyama et al. 2013, Dils et al. 2014, Hubert et al. 2015), over criteria based on the state/dynamics of the atmosphere (e.g. Wunch et al. 2011) or on representativeness area's derived from models (e.g. Oshchepkov et al. 2012), to airmass matching techniques that take into account the actual 3D/4D sensitivity of each measurement (e.g. Lambert et al. 1997,1999, Balis et al. 2007). This makes an intercomparison of the validation results difficult and it limits optimal use of the ground-based networks. To ensure reliable and traceable validation results, as required in operational validation work, community-agreed standards for co-location criteria should therefore be developed and published. Moreover, the optimal co-location strategy depends heavily on specifics such as user requirements, network coverage, instrument properties, atmospheric regimes etc. and standards should thus be diversified accordingly. As such, resolution of this gap depends to a large extent on a corresponding effort regarding gap G3.02.

Activities within GAIA-CLIM related to this gap

No attempt will be made within GAIA-CLIM to produce an authoritative document on this matter, but work within task T3.2 will contribute to the evaluation of different co-location criteria (cfr. gap G3.02), i.e. the foundation of any future recommendation or standard regarding criteria to be adopted in an (operational) validation system. Some discussion on common co-location criteria is included in D3.2 (Section 4.1).

Gap remedy

Remedy #1

Specific remedy proposed

The publication aimed for as a remedy to gap G3.02 could conclude with a set of clear recommendations, which then need to be advertised to and adopted by the different stakeholders (validation teams, space agencies defining validation requirements etc.).

Measurable outcome of success

Success is achieved when an authoritative document exists which is referred to in publications on validation results and in upcoming validation protocols.

Achievable outcomes

The technological effort on top of that required to address gap G3.02 is very small. Dissemination among and acceptance by the key stakeholders is more challenging and can probably best be achieved in the context of overarching frameworks such as the CEOS Working Group on Calibration & Validation (WGCV). The financial cost should be very low.

Relevance

This remedy directly addresses the gap. It will provide stakeholders with a traceable, authoritative reference on which to base their validation requirements and protocols regarding co-location criteria. It will also facilitate meta-analysis of different validation studies without the need to take into account differences in results due to differences in the impact of co-location mismatch on the results.

Timebound

The writing of these recommendations requires only a small amount of time (of the order of a few months, if results from G3.02 are available). However, for these recommendations to be widely adopted may require several years.

Gap risks to non-resolution

Identified future risk / impact	**Probability of occurrence if gap not remedied**	**Downstream impacts on ability to deliver high quality services to science / industry / society**
Difficulty in inter-comparing the results of validation work on related products.	High	Difficulty for the end user to choose the product most suited for his needs. Consequently also sub-optimal use of both the EO and non-satellite data sets.
Sub-optimal use of the non-satellite reference measurements.	High	Sub-optimal characterisation of the data quality, hampering the full exploitation of the capabilities of the EO system.

G3.04 Limited characterization of the multi-dimensional (spatiotemporal) smoothing and sampling properties of atmospheric remote sensing systems, and of the resulting uncertainties

Gap detailed description

Remotely sensed data are often considered as column-like or point-like samples of an atmospheric variable, e.g., WP2 assumes column and vertical profile measurements of ozone, water vapor etc. at the vertical of the station. This is also the general assumption for satellite data, which are assumed to represent the column or profile at the vertical of the satellite field-of-view footprint in case of nadir sounders, and atmospheric concentrations along a vertical suite of successive tangent points in the case of limb and occultation sounders. In practice, the quantities retrieved from a remote sensing measurement integrate atmospheric information over a tri-dimensional airmass and also over time. E.g., ground-based zenith-sky measurements of the scattered light at twilight integrate stratospheric UV-visible absorptions (by ozone, NO2, BrO etc.) over several hundreds of kilometers in the direction of the rising or setting Sun (Lambert et al., 1997). A satellite limb measurement will actually be sensitive to the atmosphere along the entire line-of-sight towards the photon source, depending on the specific emission, absorption, and scattering processes at play (e.g. von Clarmann et al., 2009). Similarly, in-situ measurements of atmospheric profiles cannot be associated with a single geo-location and time stamp, due for instance to balloon drift (e.g. Seidel et al. 2011). In a variable and inhomogeneous atmosphere, this leads to additional uncertainties not covered in the 1-dimensional uncertainties reported with the data (e.g. Lambert et al., 2011). A prerequisite for quantifying these additional uncertainties of multi-dimensional nature is not only a quantification of the atmospheric variability at the scale of the measurement (cfr. G3.01), but also a detailed understanding of the smoothing and sampling properties of the remote sensing system and associated retrieval scheme. Pioneering work on multi-dimensional characterization of smoothing and sampling properties of remote sensing systems and associated uncertainties was initiated during the last decade (e.g., in BELSPO/ProDEx projects SECPEA and A3C and in the EC FP6 GEOmon project), but in the context of integrated systems like Copernicus and GCOS, appropriate knowledge of smoothing and sampling uncertainties, still missing for several ECVs and remote sensing measurement types, has to be further developed and harmonized.

Activities within GAIA-CLIM related to this gap

Addressing this gap is a major objective of WP3, in both tasks T3.1 and T3.2. Results have already been obtained for total ozone columns, and work is ongoing for ozone, temperature, and humidity profiles, and for aerosol columns and profiles. All non-satellite instruments targeted within GAIA-CLIM are addressed. Regarding satellite data, only a selection of current missions are explored. Results will be made available in D3.4 and D3.6, and through the 'Virtual Observatory' (T3.3, D3.5 and D3.7). In the long term, this gap will require continued efforts to fully characterize the spatiotemporal smoothing and sampling properties of both new ground-based instruments and upcoming satellite sensors.

Gap remedy(s)

Remedy #1

Specific remedy proposed

Detailed modelling of the measurement process, including multi-D radiative transfer, to quantify the 4-D measurement sensitivity. An example are multi-D averaging kernels for retrieval-type measurements. If appropriate, the results from these detailed calculations can be parametrized for easy and efficient use when calculating the resulting errors and uncertainties for large amounts of data. This uncertainty calculation is done by combining the quantification of the measurement sensitivity with knowledge on the spatiotemporal variability of the atmospheric field.

Measurable outcome of success

Publications and technical notes describing for every instrument and measurement type the full 4-D measurement sensitivity, and the errors and uncertainties resulting from the assumption that a measurement can be associated with a nominal geo-location and time.

Achievable outcomes

This remedy requires a significant technical and organizational effort from the instrument teams, for which dedicated, though still relatively low (per instrument), resources are required, in particular for code modifications and additions. Addressing this gap for all instruments and ECVs that are part of e.g. the Copernicus system does represent a medium cost (i.e. between 1 and 5 M euro). Moreover, this remedy relies on the willingness of the measurement community to invest time and expertise.

Relevance

This approach represents the most comprehensive remedy to this gap, and also contributes to remedy gaps G3.02, G3.03, and G3.06.

Timebound

The time scale for full implementation of this remedy is of the order of years.

Remedy #2

Specific remedy proposed

When Remedy #1 is out of reach, a similar estimate of the multi-D measurement sensitivity can be made in a more pragmatic way based on the measurement principle and physical considerations (e.g. Lambert et al. 2011), or they can be estimated with empirical methods.

Measurable outcome of success

As for Remedy #1

Achievable outcomes

As opposed to Remedy #1, this more pragmatic approach does not require direct involvement by the measurement teams and the cost estimate is significantly lower.

Relevance

While not as comprehensive and accurate a solution as Remedy #1, it would in many cases already allow a good characterization of the (uncertainties resulting from) the measurement smoothing and sampling properties, and therefore be of great value in the context of validation and to close gap G3.06.

Timebound

Development and first exploitation of these pragmatic "observation operators" can typically be done in less than a year with an investment of 1 FTE.

Gap risks to non-resolution

Identified future risk / impact	**Probability of occurrence if gap not remedied**	**Downstream impacts on ability to deliver high quality services to science / industry / society**
Incomplete total measurement uncertainty budget, in particular when comparing with measurements or models with differing sampling and smoothing.	High	Incomplete data characterization and potentially limited or flawed interpretation of validation results.

G3.05 Representativeness uncertainty assessment missing for higher-level data based on averaging of individual measurements

Gap detailed description

The creation of level-3 (and level-4) data by averaging non-uniformly distributed measurements inevitably leads to representativeness errors, see e.g. Coldewey-Egbers et al., (2015) for the case of a level-3 (gridded monthly means) total ozone data set. The resulting representativeness uncertainty can be larger than the formal uncertainty on the mean. However, estimates of these representativeness uncertainties are rarely included with the data product. Also, the representativeness of the ground-based network should be taken into account when validating such data sets, i.e. the sparse spatial and temporal sampling of the ground network leads to significant representativeness uncertainties in the derived monthly (zonal) means.

Also, in the context of validation of level-2 data, measurements are sometimes averaged after co-location (e.g. Valks et al., 2011, Schneising et al.,2012) without explicit calculation of the representativeness errors and resulting uncertainty.

Activities within GAIA-CLIM related to this gap

No work in this direction is foreseen within GAIA-CLIM.

Gap remedy(s)

Remedy #1

Specific remedy proposed

Studies quantifying the representativeness of averages, e.g. by model-based simulations of averages based on either the limited real sampling or on an ideal, complete sampling. More pragmatically, representativeness uncertainties can also be computed as a function of parametrized measurement inhomogeneity and field variability (Sofieva et al., 2014).

Measurable outcome of success

Success is achieved when level-3 data sets include not only the formal uncertainty on the mean and the variance around that mean, but also an estimate of the representativeness uncertainty on that mean. The reliability of this reported representativeness uncertainty must than also be validated, e.g. with targeted intensive field campaigns.

Achievable outcomes

Technological effort required to address this gap depends on the particular product and on whether atmospheric variability is well understood for that ECV (cfr. gap G3.01). For most of the ECVs targeted by GAIA-CLIM, an estimate of the representativeness uncertainty should be achievable at a low cost. The additional validation required to assess the quality of this representativeness uncertainty estimate may –in absence of existing reference data sets at sufficiently high spatial and temporal sampling– require a more significant investment, e.g. to conduct intensive field campaigns.

Relevance

This remedy offers a comprehensive solution to the gap.

Timebound

The calculation of representativeness uncertainties is not time consuming and can be done on a time scale of weeks or months. For this to become common practice among data product creators may take several years.

Gap risks to non-resolution

Identified future risk / impact	Probability of occurrence if gap not remedied	Downstream impacts on ability to deliver high quality services to science / industry / society
Representativeness uncertainties unknown and unreported.	Very high	Potential over-interpretation of the data due to representativeness uncertainty not being taken into account.

G3.06 Missing comparison error/uncertainty budget decomposition including errors/uncertainties due to sampling and smoothing differences

Gap detailed description

Ideally, every validation exercise based on comparisons with ground-based reference data should investigate whether the comparison statistics (bias or mean difference, spread on the differences, drift, etc.) are compatible with the reported random and systematic measurement uncertainties, while taking into account the additional uncertainties due to spatiotemporal sampling and smoothing differences, i.e. non-perfect co-location of the airmasses sensed by both instruments. Indeed, only in a few particular cases is it possible to adopt co-location criteria that result in a sufficiently large number of co-located pairs, while at the same time keeping the impact of atmospheric variability on the comparisons (due to spatiotemporal mismatches) well below the measurement uncertainties. In all other cases, the discrepancy between two data sets will contain non-negligible terms arising from sampling and smoothing differences, which need to be taken into account. In fact, such an analysis is essential to fully assess the data quality and its fitness-for-purpose, but in practice, it is rarely performed. Some pioneering work was published by Cortesi et al. (2007) on uncertainty budget closure for MIPAS/ENVISAT ozone profile validation, by Ridolfi et al. (2007) for the case of MIPAS/ENVISAT temperature profiles validation, by Fasso et al. (2013) in the context of radiosonde intercomparisons, and by Verhoelst et al. (2015) for GOME-2/MetOp-A total ozone column validation. However, no such studies have hitherto been performed for most other ECVs and/or instruments.

Activities within GAIA-CLIM related to this gap

This gap is a key focal point for tasks T3.1 and T3.2 in WP3. Dedicated studies will aim for full error (or uncertainty) budget decomposition for representative comparison exercises, involving all non-satellite measurement types targeted by GAIA-CLIM and several current satellite sounders. Moreover, some of these results will be transferred into the Virtual Observatory to allow end users to also decompose the uncertainty budget of their comparisons.

Gap remedy(s)

Remedy #1

Specific remedy proposed

Observing System Simulation Experiments (OSSEs), such as those performed with the OSSSMOSE system by Verhoelst et al. (2015) on total ozone column comparisons. These are based on a quantification of the atmospheric field and its variability (cfr. gap G3.01), e.g. in the shape of reanalysis fields, and of the sampling and smoothing properties of the instruments that are being compared (cfr. gap G3.04). The aim is to calculate the error due to spatiotemporal mismatch for each comparison pair, and to derive the mismatch uncertainties from these, so that they can be added to the measurement uncertainties to derive the full uncertainty budget.

Measurable outcome of success

At a high level, success is achieved when validation (and other comparison) results are published including a full uncertainty budget decomposition, taking into account spatiotemporal mismatch uncertainties. Or when they include a convincing demonstration that mismatch uncertainties are well below the measurement uncertainties and are therefore negligible.

At a lower level, success is achieved if the OSSE allows one to close the uncertainty budget, i.e. the measured differences (or their statistics) are compatible with the sum of all uncertainty sources. Note that this requires reliable measurement uncertainties as well.

Achievable outcomes

The technological and organizational challenges are mostly related to the underlying gaps G3.01 and G3.04. When these are properly addressed, the calculation of the full uncertainty budget of a comparison exercise requires only a low investment in time (less than a year) and resources (less than 1 FTE).

Relevance

This remedy comprehensively addresses the gap.

Timebound

Performing the OSSE for a specific validation/comparison exercise requires only a small amount of time (order of months), but the development and scientific assessment of the building stones (high-resolution atmospheric fields and observation operators quantifying the true 4-D measurement sensitivity) can take years of effort (cfr. gaps G3.01 and G3.04).

Remedy #2

Specific remedy proposed

To compute an uncertainty budget based on the heteroskedastic functional regression approach, which is named STAT4COLL, for each ECV/instrument comparison for the selected/available datasets. As a result mismatch uncertainties are obtained from statistical modelling, so that they can be added to the measurement uncertainties to provide the full uncertainty budget.

Measurable outcome of success

As for remedy #1

Achievable outcomes

The technological/organizational viability is considered medium and the cost is estimated low. Nonetheless, challenges are still related to the insufficient number of reference measurement available to precisely address the proposed gap for some ECV/instrument comparisons.

Relevance

GAIA-CLIM will approach this gap using advanced statistical approaches whose application may be generalized and extended to other ECVs. As a post GAIA-CLIM development, integration between remedy #1 and #2 could have a big potential in instrument comparisons.

Timebound

Performing STAT4COLL for a specific validation/comparison exercise requires only a limited amount of time (approximately one year).

Gap risks to non-resolution

Identified future risk / impact	**Probability of occurrence if gap not remedied**	**Downstream impacts on ability to deliver high quality services to science / industry / society**
Incorrect (or at least incomplete) feedback from validation work on data quality.	High	Poorly qualified data quality. Potential of the EO system not maximized.

5. Summary

Currently, great effort is being invested upon improving the performance of the ground-based networks. This will support the provision of a comprehensive set of reference measurements and will play a key role in ensuring the fitness-for-purpose of the atmospheric EO system to monitor climate change and air quality. Areas of focus include: network coverage, measurement traceability, (fast) data delivery, and uncertainty characterization and communication (e.g. within the EC FP7 and H2020 projects GAIA-CLIM, QA4ECV, FIDUCEO). An additional topic requiring community-wide investment arises when these reference measurements are co-located and compared with the satellite data to be validated: the impact of co-location mismatch, i.e. differences in smoothing and sampling of the variable and inhomogeneous atmosphere between non-satellite and satellite data. These differences lead to additional errors and uncertainties in the comparison results, and must be minimized and/or quantified to ensure both optimal use of the reference measurements and reliable feedback on satellite data quality. While some exploratory research exists for a few atmospheric ECVs (temperature, water vapour, ozone, NO_2, and aerosol properties) and instruments, a more comprehensive knowledge base must be established, that is mature enough to be integrated into an operational context, such as the Copernicus programme. This is to include other trace gases and aerosols, covering specific aspects such as the definition of optimal co-location criteria, the development and application of methods to quantify the uncertainties resulting from mismatch, the quantification of the representativeness of a single station and a network, etc. With regard to the upcoming Sentinel missions, this need exists in particular for ozone, NO_2, HCHO, CO, CH_4, SO_2 and aerosol load (Sentinel-4, Sentinel-5p, and Sentinel-5).

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Glossary

CEOS	Committee on Earth Observation Satellites
ECV	Essential Climate Variable
ECMWF	European Centre for Medium-Range Weather Forecasts
FIDUCEO	Fidelity and Uncertainty in climate records for Earth Observations
FTE	Full time equivalent
GRUAN	GCOS Reference Upper-Air Network
GSICS	Global Space based Inter-Calibration System
GNSS-RO	Global Navigation Satellite System - Radio Occultation
IASI	Infrared Atmospheric Sounding Interferometer
MIPAS	The Michelson Interferometer for Passive Atmospheric Sounding
MODIS	Moderate Resolution Imaging Spectroradiometer
OSSE	Observing System Simulation Experiment

OSSSMOSE	Observing System of Systems Simulator for Multi-mission Synergies Exploration
QA4ECV	Quality Assurance for ECV
UAV	Unmanned Aerial Vehicle
WIGOS	WMO Integrated Global Observing System