Guide to Uncertainty in Measurement & its Nomenclature

Version 4.0

GAIA-CLIM
Gap Analysis for Integrated
Atmospheric ECV Climate Monitoring
Mar 2015 - Feb 2018

A Horizon 2020 project; Grant agreement: 640276

Date: 30 November 2017

Dissemination level: PU

Work Package 2; Compiled by Paul Green &
Tom Gardiner (NPL)

Work-package	WP2 (Measurement uncertainty quantification)
Deliverable	D2.6
Title	WP2 Guide to Uncertainty in Measurement & its Nomenclature
Nature	R
Dissemination	PU
Lead Beneficiary	National Physical Laboratory, UK
Date	30 November 2017
Status	Final
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Version history

Version	Principal updates	Owner	Date
1.0	First release	NPL	18.09.2015
1.1	Revision of Annex A & addition of §7	NPL	05.11.2015
2.0draft	Addition of §8 and minor changes in §7	NPL	18.11.2016
2.0	Addition of §8.1.2	NPL	18.01.2017
3.0	Revisions to §7.2, §8.1 & §8.2. Changing the element contribution & summary tables and adding example chains.	NPL	18.05.2017
4.0draft	Additional guidance on the Traceability Chain Shapes and Definitions in §7.2. The measurement function/equation section added. Reference & annex sections swapped. Example PTUs added as annex B-F	NPL	24.11.2017
4.0	Deliverable D2.6	NPL	30.11.2017

The content of sections 1-6 of this guidance note are largely taken from the 'Intermediate Uncertainty Analysis for Earth Observation: Instrument Calibration Module' course notes [1]

1 The ISO and BIPM Guide to the Expression of Uncertainty in Measurement (GUM)

The *Guide to the Expression of Uncertainty in Measurement*, known as 'the GUM', provides guidance on how to determine, combine and express uncertainty [2]. It was developed by the JCGM (Joint Committee for Guides in Metrology), a joint committee of all the relevant standards organisations (e.g. ISO) and the BIPM (*Bureau International des Poids et Mesures*). This heritage gives the GUM authority and recognition. The JCGM continues to develop the GUM and has recently produced a number of supplements. All of these, as well as the 'VIM' (International Vocabulary of Metrology, [3]) are freely downloadable from the BIPM website[1].

2 Measurement Traceability and SI

Measurement traceability is defined by the Committee for Earth Observation Satellites (CEOS) as the

> *Property of a measurement result relating the result to a stated metrological reference (free definition and not necessarily SI) through an unbroken chain of calibrations of a measuring system or comparisons, each contributing to the stated measurement uncertainty.*

Measurement traceability is an unbroken chain (i.e. it is calibrated against X, which was calibrated against Y, which was calibrated against Z, all the way back to SI, or, perhaps, a recognised authoritative reference). Additionally, effective quality assurance requires the documentary evidence that each step is done in a reliable way (ideally audited, at least thoroughly peer-reviewed). Validation of datasets, a prime concern of the GAIA-CLIM project, requires the combination of measurement traceability, quality assurance & process traceability of the reference & target measurement systems; providing an unbroken chain between the measurement systems through a common measurand, be that the target geophysical parameter or a closely related quantity.

Measurement traceability should, ideally, be to the International System of Units, known as the SI from its French name, *le Système international d'unités*. The SI units provide a coherent system of units of measurement built around seven base units and coherent derived units. A coherent system of units means that a quantity's value does not depend on how it was measured. The SI is an evolving system, with the responsibility for ensuring long term consistency with the General Conference on Weights and Measures (CGPM), run through the International Bureau of Weights and Measures, the BIPM, and maintained nationally through the National Metrology Institutes (NMIs). The CIPM Mutual Recognition Arrangement (CIPM MRA) signed in 1999 between the NMIs ensures that measurements made traceably to any NMI within the CIPM MRA are recognised by other NMIs. This is enforced by both formal international comparisons and a process of auditing and peer-reviewing statements of calibration capability. For the user, this means that traceability to the SI can be achieved through any NMI within the CIPM MRA.

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[1] http://www.bipm.org/en/publications/guides/

3 The measurement function/equation

One approach to uncertainty analysis and metrological traceability is to start with the measurement function. The VIM 2008 formally defines a measurement function as:

a function of quantities, the value of which, when calculated using known quantity values for the input quantities in a measurement model, is a measured quantity value of the output quantity in the measurement model.

where,

the measurement model is the mathematical relation among all quantities known to be involved in a measurement.

Here the word "measurement" must be considered in its broadest sense and includes the concept of an indirect measurement, where an indicated quantity (e.g. a signal count) is transformed to the measurand (e.g. brightness temperature), which is the quantity intended to be measured.

The measurement function is defined from the measurement model which establishes the mathematical relations between the input quantities. Input quantities are, for example, the counts and the calibration coefficients. Note that this concept is also often known as the "measurement equation". Here we use the word "function" in the most general sense. For the sensors under consideration we can explicitly write the measurement function in terms of an analytic expression. In other cases, the measurement function is defined by e.g. the iterative solution of a measurement model through code.

We perform our uncertainty analysis by considering the different input quantities to the measurement function. Each input quantity may be influenced by one or more error effects, each of which has an associated probability distribution and our aim is to establish the probability distribution of the output quantity. In a processing (or metrological traceability) chain there will be a series of such combinations, where the output quantity of one stage becomes an input quantity of the next stage.

Note that we should also consider the extent to which the measurement function describes the true physical state of the instrument. We usually account for this by including a term zero. This explicitly represents effects expected to have zero mean that are not captured by the measurement function (i.e. there is an uncertainty associated with this quantity being zero). Therefore we write the measurement function as:

$$Y = f\left(X_1, X_2, \ldots, X_N\right) + 0. \qquad (1)$$

Uncertainty analysis is based on the relationship between the measurand (measured value) and various input quantities embodied in a measurement function. Each input quantity may be influenced by one or more error effects, each of which has an associated probability distribution.

The Guide to the Expression of Uncertainty in Measurement [2], provides guidance on how to determine, combine and express uncertainty. The GUM and its supplements describe both the Law of Propagation of Uncertainty and Monte Carlo methods as methods to propagate uncertainties from the input distributions to the measurand error distribution.

Monte Carlo methods approximate the input probability distributions by finite sets of random draws from those distributions and propagate the sets of input values through the measurement function to obtain a set of random draws from the output probability distribution. The output values are then analysed statistically, for example to obtain expectation values, standard uncertainties and error covariances. The measurement function in this case need not be linear nor written algebraically. Steps such as inverse retrievals and iterative processes can be addressed. The input probability distributions can be as complex as desired, and can include digitised distributions, where signals are digitised for on-board recording and transmission.

3.1 Hierarchical uncertainty analysis and effects

An uncertainty analysis centred on the measurement function is used to calculate a measurand from input quantities. Some of these input quantities will be directly measured, others may be determined through their own measurement function, with input quantities that are directly measured or determined through another measurement function.

At the end of each ‘branch’ of this hierarchical structure is a quantity that is directly estimated: through measurement, through modelling or through data analysis. And each such quantity will be sensitive to a number of effects, each of which has an associated uncertainty that can itself be estimated through measurement, through modelling or through data analysis. In our measurement functions we always include a term “+ 0” which represents effects relating to the assumptions underlying the form of the measurement function (e.g. that it is quadratic). Uncertainty analysis starts at the effects and propagates these through each measurement equation (perhaps several through the hierarchy). Almost all quantities in the measurement equation will have one or more associated effects, with the exception of mathematical and physical constants and a small number of other terms used either as indicators or as agreed references.

Uncertainty analysis assumes that the result of a measurement has been corrected for all recognized significant systematic effects and that every effort has been made to identify such effects. This effectively means that the measurand will be as accurate as possible given the current state of knowledge. When we perform analyses at the effects level we need to decide whether the effect could be fully, or partially corrected for, and if so we should apply the correction. The residual effect uncertainty is the uncertainty associated with the correction. The metrological thinking involved in performing uncertainty analysis therefore often has the unexpected side effect of improving the ECV product as effects are corrected for.

4 Errors, uncertainties and corrections

The terms ‘error’ and ‘uncertainty’ are not synonyms, although they are often confused in EO applications. To understand the distinction, consider the result of a measurement – the measured value. The value will differ from the true value for several reasons, some of which we may know about. In these cases, we may be able to identify and apply a **correction**. A correction is applied to a measured value to account for known differences, for example the measured value may be multiplied by a gain determined during the instrument’s calibration, or a measured optical signal may have a dark reading subtracted. This correction will never be perfectly known and there will also be other effects that cannot be corrected, so after correction there will always be a residual, unknown **error** – an unknown difference between the measured value and the (unknown) true value.

The specific error in the result of a particular measurement cannot be known, but we describe it as a draw from a probability distribution function. The **uncertainty** associated with the measured value is a measure of that probability distribution function; in particular, the **standard uncertainty** is the standard deviation of the probability distribution, and the equivalent of this for other distributions. There are generally several ‘sources of uncertainty’ that jointly contribute to the uncertainty associated with the measured value. These will include uncertainties associated with the way the measurement is set up, the values indicated by instruments, and residual uncertainties associated with corrections applied. The final (unknown) error on the measured value is drawn from the overall probability distribution described by the uncertainty associated with the measured value. This is built up from the probability distributions associated with all the different sources of uncertainty.

The use of the words ‘error’ and ‘uncertainty’ described here is consistent with paragraph 2.2.4 of the GUM, and described graphically in Figure 1.

Conversely it is worth considering what is *not* a measurement uncertainty:

- Mistakes made by operators are not measurement uncertainties. They should generally be avoided, and identified thorough checking of the results obtained.
- Tolerances are not uncertainties. They are acceptance limits which are chosen for a process or a product.
- Specifications are not uncertainties. A specification tells you what you can expect from a product or what a user requires from a product. It may be very wide-ranging, including ‘non-technical’ qualities of the item, such as its appearance. Specifications may or may not be attainable.

5 The law of propagation of uncertainties

The aim of any uncertainty analysis is to estimate the uncertainty associated with the measured value, which may be the result of a process involving several different parameters being controlled and set or measured, and a calculation. To obtain the final uncertainty, uncertainties due to *each and every* element in the process that affect the final result must be combined – i.e. they must be propagated through this process. Ref [1] contains an extended worked example for an airborne EO instrument.

The GUM gives the Law of Propagation of Uncertainty as,

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

which applies for a measurement model of the form

$$Y = f(X_1, X_2, X_3, \ldots, X_i, \ldots) \tag{3}$$

where an estimate x_i of quantity X_i has an associated uncertainty $u(x_i)$. The quantity $u_c^2(y)$ is the squared standard uncertainty (standard deviation of the probability distribution) associated with the measured value y which comes from a combination of the uncertainties associated with all the different effects, x_i. The square of the standard uncertainty is also known as the **variance**. The second term on the right hand side of eqn. 2 sums the covariance terms. The covariance is a measure of the uncertainty common to the two quantities in the measurement model.

It can help to write the Law of Propagation of uncertainties in terms of **sensitivity coefficients** as

$$u_c^2(y) = \sum_{i=1}^{n} c_i^2 u^2(x_i) + 2\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} c_i c_j u(x_i, x_j), \quad (4)$$

where the sensitivity coefficient $c_i = \partial f / \partial x_i$. The sensitivity coefficient is a 'translation' from one variable to another. It answers the question: "how sensitive is y to an uncertainty associated with x_i ?"

The law of propagation of uncertainties is written in this slightly complex notation of two parts to separate two terms:

- The first term is the sum of the squares of the standard uncertainties $u(x_i)$ (the sum of the variances) associated with each individual effect multiplied by the relevant **sensitivity coefficient** (the partial derivative). This first term is what is meant by the description '**adding in quadrature**'.
- The second term deals with the **covariance** of correlated quantities. The covariance is a measure of how much the two quantities vary together. If the covariance term is zero, this term becomes zero by definition.

Note that the covariance term covers all pairs of different quantities, e.g. $(x_1, x_2), (x_1, x_3), (x_2, x_3), \ldots$ Since the covariance $u(x_1, x_2) = u(x_2, x_1)$, the summation is only over the combinations where $i < j$ (i.e. only half the cases). The 2 in front of this term accounts for the opposite cases.

5.1 Coverage factor k

Having scaled the components of uncertainty consistently, to find the combined standard uncertainty, we may then want to re-scale the result. The combined standard uncertainty may be thought of as equivalent to 'one standard deviation', but we may wish to have an overall uncertainty stated at another level of confidence, e.g. 95 percent. This re-scaling can be done using a coverage factor, k. Multiplying the combined standard uncertainty, u_c , by a coverage factor gives a result which is called the expanded uncertainty, usually shown by the symbol U,

$$U = k.u_C \quad (5)$$

A particular value of coverage factor gives a particular confidence level for the expanded uncertainty. Most commonly, we scale the overall uncertainty by using the coverage factor k = 2, to give a level of confidence of approximately 95 percent. (k = 2 is correct if the combined standard uncertainty is normally distributed. This is usually a fair assumption, but the reasoning behind this is explained elsewhere, in [2].) Some other coverage factors (for a normal distribution) are:

- k = 1 for a confidence level of approximately 68 percent
- k = 2.58 for a confidence level of 99 percent
- k = 3 for a confidence level of 99.7 percent

Other, less common, shapes of distribution have different coverage factors. Conversely, wherever an expanded uncertainty is quoted with a given coverage factor, you can find the standard uncertainty by the reverse process, i.e. by dividing by the appropriate coverage factor.

6 Classifications

Random and Systematic Effects

Correlation will be introduced whenever there is something in common between two measured values that will be combined (i.e. two values that will be averaged, or two quantities used in a measurement equation, or values at different wavelengths that will be combined through interpolation or integration). The simplest way to describe this is in terms of random and systematic effects.

Random effects are those that are not common to the multiple measurements being combined. A typical example is noise: two measured values may both suffer from noise, but the effect of noise will be different for each of the two measured values (for example, if noise has increased one measured value, this provides no information about whether any other measured value is increased or decreased by that noise, nor by what extent).

Systematic effects are those that are common to all measured values. If one measured value has been increased as a result of a systematic effect, then we can make a reliable prediction regarding whether any other measured value will be increased, and by how much. For example each time the distance is set for an irradiance measurement using a particular lamp, there will be a (normally small) error in that distance. This will equally affect all measurements of that lamp until the next alignment. If multiple measured values are averaged without realignment, or measured values at different wavelengths are combined in an integral, then the distance error will be common to all those measured values. This is a systematic effect.

When validating EO datasets correlated systematic effects common to both the reference & target instrument systems may exist. For instance, SZA, surface albedo and background atmospheric absorption & scattering processes may be common uncertainty contributors to both measurement systems.

Some effects, such as noise, are always random; other effects can be either random or systematic depending on the measurement process. There may be additional uncertainty types, such as structured random, which will be systematic over one timescale, but effectively random over longer timescales. For example, if three measured values of a lamp are combined in an average and the lamp is realigned between each measurement, then alignment/distance is a random effect. If the lamp is not realigned between measurements, then alignment/distance is a systematic effect.

The error in the measured value due to a random effect will change from one measured value to another. In this case the uncertainty associated with the effect may be the same for each measured value (the probability distribution for the effect is the same for each measured value), but each measured value is independent of each other measured value, as influenced by this effect. The unknown random error at each measured value is an independent draw from the probability distribution, meaning that the error due to the random effect is not only different from, but also independent of, the error at any other wavelength. The standard uncertainty associated with random effects is usually (but not always) determined by calculating the standard deviation of repeated measured values.

Such repeat measurement is difficult, if not impossible, in the atmospheric domain as the measured quantity is almost invariably non-static. In a few cases pseudo repeat measurements are possible, that is, if measurements can be taken sufficiently close in time and space and also close in sensitivity, so that the contribution of natural variability to the obtained standard deviation becomes negligible. But those cases are not the rule and in general any estimate of the standard deviation will include contributions from spatial, temporal and sensitivity mismatch.

Another important consideration in the atmospheric domain are influence quantities. Influence quantities do not affect the instrument measurand directly, but affects the derived geophysical measurand through departure from the assumptions of the processing model; e.g., cloudiness in the field-of-view of an instrument can influence the accuracy of its measurement.

The error in the measured value due to a systematic effect will be the same from one measured value to another. The uncertainty associated with the effect is the same for each measured value and the error is the same draw from the probability distribution for all measured values. The standard uncertainty associated with systematic effects cannot be determined by repeat measurements, unless the effect is intentionally altered between repeats (e.g. by realigning a source multiple times using a series of different ‘extreme but acceptable’ alignments in an experiment to characterise the impact of source alignment).

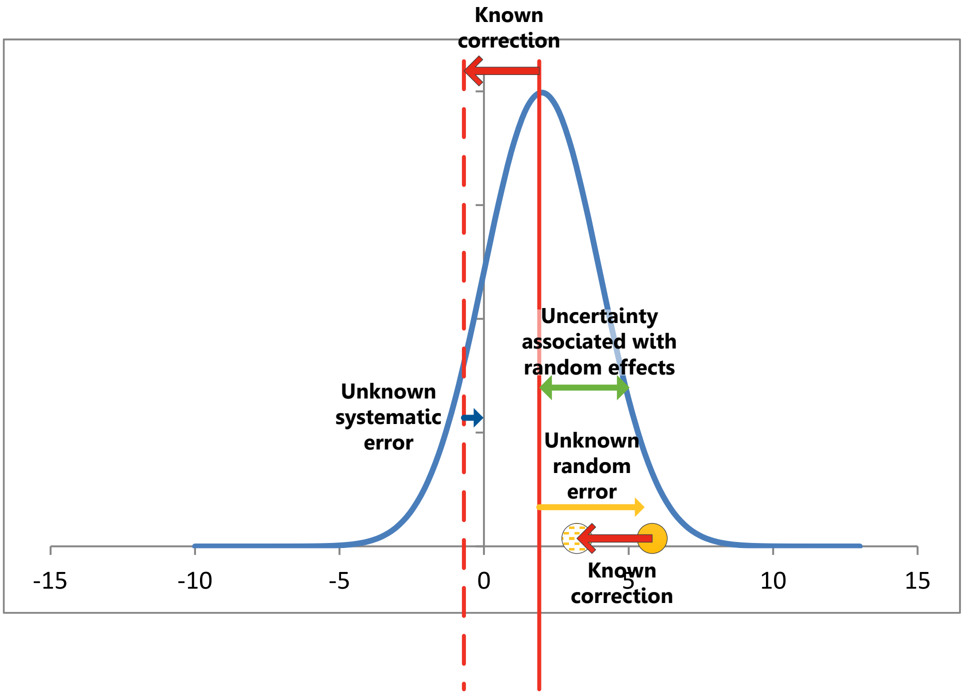

Figure 1: Representing a measurement where there is a known correction, an unknown systematic effect and random effects.

Figure 1 represents a measurement process where there is a known correction, an unknown systematic effect and random effects.

- A measurement is made (obtaining the value represented by the golden circle).
- We know of a correction – a systematic bias due to, e.g. a dark reading – and apply this correction, obtaining the value of the flecked circle.
- There is still an unknown error from the true value of zero. If we make many measurements we obtain the probability distribution function shown in blue. The spread of this, the standard deviation of the normal distribution, is the standard uncertainty associated with random effects – those effects that change from measurement to measurement. Our measured value is a draw from this probability distribution function. If we take multiple measurements we obtain different draws. The average will tend towards the value at the peak of this distribution.
- When the known correction is applied, the result will be close to the true value, but differ from it by an unknown systematic error common to all the measured values. This comes from its own probability distribution function and all measured values have the same draw from that distribution (not shown in the figure, but this will take the form of a probability distribution centred at the true value with a standard deviation equal to the uncertainty associated with systematic effects).

6.1 Type A and Type B

The terms ‘Type A’ and ‘Type B’ are used with uncertainty analysis. This use comes from the GUM, which defines:

- **Type A evaluation (of uncertainty)** method of evaluation of uncertainty by the statistical analysis of series of observations
- **Type B evaluation (of uncertainty)** method of evaluation of uncertainty by means other than the statistical analysis of series of observations

Type A evaluation uses statistical methods to determine uncertainties. Commonly this means taking repeat measurements and determining the standard deviation of those measurements. This method can only treat uncertainties associated with random effects, for example the uncertainty associated with measurement noise.

Type B evaluation uses 'any other method' to determine the uncertainties. This can include estimates of systematic effects from previous experiments or the scientist's prior knowledge. It can also include random effects determined 'by any other method'. For example we may model room temperature by a random variable in the interval from 19 °C to 21 °C – the temperature range of the air-conditioning settings. Similarly, we may say that a voltmeter with 2 digits after the decimal place has an uncertainty associated with resolution of 0.005 V because we know the rounding range.

It is common to assume that ‘Type A’ evaluation is for random effects and ‘Type B’ evaluation is for systematic effects. This is generally, but not always, the case. For example, a ‘Type A’ method may be used to determine the uncertainty associated with alignment: a lamp may be realigned ten times and the standard deviation of those ten measurements used to determine an uncertainty associated with alignment. In a later experimental set-up, measurements may be taken at multiple wavelengths and these combined in a spectral integral. For that integral, alignment is a systematic effect (the lamp is not realigned from wavelength to wavelength) even though the determination of the associated uncertainty was performed using ‘Type A’ methods. Similarly, the uncertainty associated with a random effect may be estimated from prior knowledge, or a measurement certificate, and thus by a ‘Type B’ method.

Is it worth noting that field measurements of atmospheric properties will typically have a lot of type B uncertainties and that a comprehensive uncertainty analysis would involve several quantities not quantifiable in a lab setting.

6.2 Absolute and relative uncertainties

The uncertainties given in the law of propagation of uncertainties by the symbol $u(x_i)$ are always standard absolute uncertainties. The term **standard uncertainty** means that it is a single standard deviation of the probability distribution function associated with that quantity. The term **absolute uncertainty** means that it has the same unit as the measurand. In other words, if the signal is in volts, the absolute uncertainty will also be in volts. If the distance is in metres, the absolute uncertainty will also be in metres.

It is common in radiometric calibrations to describe **relative uncertainties**, with units of percent. The relative uncertainty is the absolute uncertainty divided by the quantity, i.e. $u(x_i)/x_i$.

7 Writing about uncertainties

In casual language we talk about 'averaging a set of measurements' or 'the uncertainty in the measurement is 0.5 %'. In metrology these words are defined carefully to reduce misunderstanding. We cannot 'average a set of measurements' but we can 'average the measured values' obtained from those measurements. The measurement has no uncertainty, there is an uncertainty *associated with* the measured value. For a non-specialist, such definitions can seem pedantic, as with jargon in all fields; but for a specialist, such careful use of words is a source of clarity. The words are defined through the VIM: the international vocabulary of metrology [3].

A *measurement* is made (instruments set up and value recorded) of a *measurand* (a quantity, such as radiance) to obtain a *measured value* (e.g. 0.5 W m^{-2} sr^{-1} nm^{-1}) with an *associated uncertainty* (e.g. 0.5 %). The VIM defines **measurement** as the

> *process of experimentally obtaining one or more quantity values that can reasonably be attributed to a quantity*

The most important word here is *process*: it defines measurement as the act of measuring. A measurement is not a quantity nor a result. The VIM defines **measurand** as the

> *quantity intended to be measured*

In turn, **quantity** is the

> *property of a phenomenon, body or substance, where the property has a magnitude that can be expressed by a number and a reference.*

Thus quantities are things like length, mass, reflectance, irradiance, instrument gain, etc. When you measure a quantity, that quantity is the measurand of the measurement. The **measurement result** is defined by the VIM as the

> *set of quantity values being attributed to a measurand together with any other available relevant information*

The "other available relevant information" refers to the associated uncertainty, perhaps expressed directly, perhaps as a probability density function, or perhaps implied by the number of digits provided with the result (the latter providing less reliable information). The **quantity value** is a

> *number and reference together expressing magnitude of a quantity*

The reference usually means the unit. The **measured quantity value** (often shortened to measured value) is the quantity value that is the particular measurement result.

A fuller glossary of term is given in Appendix A, see the VIM [5] for the full list of terminology.

8 Framework for the production of metrological robust traceability & process chains

Key to understanding and expressing the robust uncertainty analysis of any atmospheric data product is the ability to clearly display the processing steps taken to produce the dataset. As discussed earlier, to obtain the final uncertainty, uncertainties due to *each and every* element in the process that affect the final result must be combined – i.e. they must be propagated through this process. One method for achieving such a detailed understanding is developing a traceability chain. In metrology, the aim of developing a traceability chain is to demonstrate the series of calibrations which link a measurement to a reference standard. For atmospheric applications, this needs to be developed much further to allow processes to be captured in detail.

Following the procedure of other QA frameworks developed for essential climate variables (ECVs) [6], the total chain is divided into two components that reflects the division between

- Instrument processing chain to L0 instrument raw data – physical model
- Data processing chain from L0 instrument data to final geophysical parameter – processing model.

8.1 Types of Traceability Chains

Regardless of the process being considered (instrumental or data processing), a framework of traceability models is currently being developed within the QA4ECV project [6] that is being trialled within sister projects, such as FIDUCEO [7]. These are not hard & fast rules that should be blindly followed, but a method conceived to help the user think about all the contributions to the uncertainty budget. As the framework is still being developed, it is hoped that its evolution will be guided via feedback from the user community, including GAIA CLIM. This framework involves considering the traceability in terms of three models.

1. **Physical Model** – This model considers the real-world situation, i.e. what is actually occurring in the real world and the physics driving this.
2. **Processing Model** – This model considers how the raw data collected is processed to provide the end product, through calibration to the final geophysical parameter.
3. **Metrological Model** – This model considers the calibration, or linkage, of a measurement or processed data to a reference.

Separating the types of traceability chain into these three models provides several advantages: the separation essentially provides three angles from which the problem can be approached, it allows for the persons producing the chains to have a clear set of boundaries in which to operate when considering the production of the chains as well as being able to choose the type of model with which they are the most familiar as a starting point. It is noted that there may be significant overlap between the models.

8.1.1 Physical Model

The physical model chains describe the real-world by considering the physics behind each stage of the process which contributes to the measurements taken. This includes all of the physical processes associated with the measurand detection; for a radiometric instrument, this covers the physics of how the EM radiation enters the instrument, how it is modified by the optical system, how it is detected and how it is converted to an electrical signal which makes up the output raw signal.

The aim of the physical model is to be able to describe, reliably, the physical processes which contribute to the generation of the L0 data. Therefore, obtaining a suitable physical model requires an understanding of the detector physics including sources of uncertainty such as noise, the non-linearity of a detector, the Spectral Response Function (SRF) of the detector etc. The model would also include any processing of the signal undertaken by the instrument itself, for example, data compression.

It is unlikely that the physical model chain would incorporate *all* of the possible physical processes occurring in the real-world situation due to the complexity of the real-world. The physical model would essentially represent a simplified "best guess" of the real-world. However, in producing the physical model, all contributions should be considered and those processes not included in the model, potentially as they are deemed to have a negligible effect on the data product should at least be documented.

Figure 2 shows an example instrument model for a satellite sensor, showing the main physical processing steps from the incoming radiation to the L0 data.

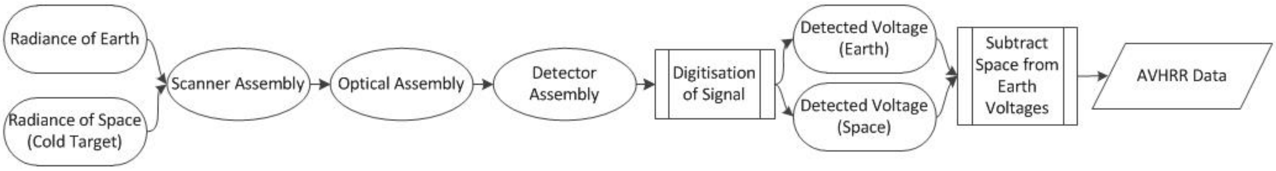

Figure 2: Physical Chain Example – AVHRR Instrument

8.1.2 Processing Model

The processing model chains are intended to describe the input data, processes and output data that contribute to an overall geophysical parameter generation from both Level 0 and ancillary data. This model will include all the processes and assumptions built into the calibration algorithm, as well as any external models or ancillary data used. The processing model will describe a series of calculation steps that the data undergoes to obtain the measurand of interest (i.e. equations and computational models), with inputs derived from the previous step or from pre-set parameters and coefficients, and an output that leads to the next step in the processing chain.

This chain type is conceptually the easiest to understand, particularly within the EO community, where a data producer would intuitively think of a traceability chain as the steps required to produce their product or undertake their process.

One of the key advantages of producing both physical & processing models is the ability to compare these models, and in so doing identify differences between the two. This would effectively give the data / product producers details of how their modelled world (represented by the processing chain) differs from the real-world (represented by the physical chain).

An example process chain diagram of algorithm traceability is shown in Figure 3. Further examples of traceability chains developed within the QA4ECV project can be found at http://www.qa4ecv.eu/ecvs

At a basic level the diagram would contain central boxes representing the processing steps. In addition more detailed information about that step in terms of basic documentation, provenance, assumptions employed and uncertainty analysis should also be provided.

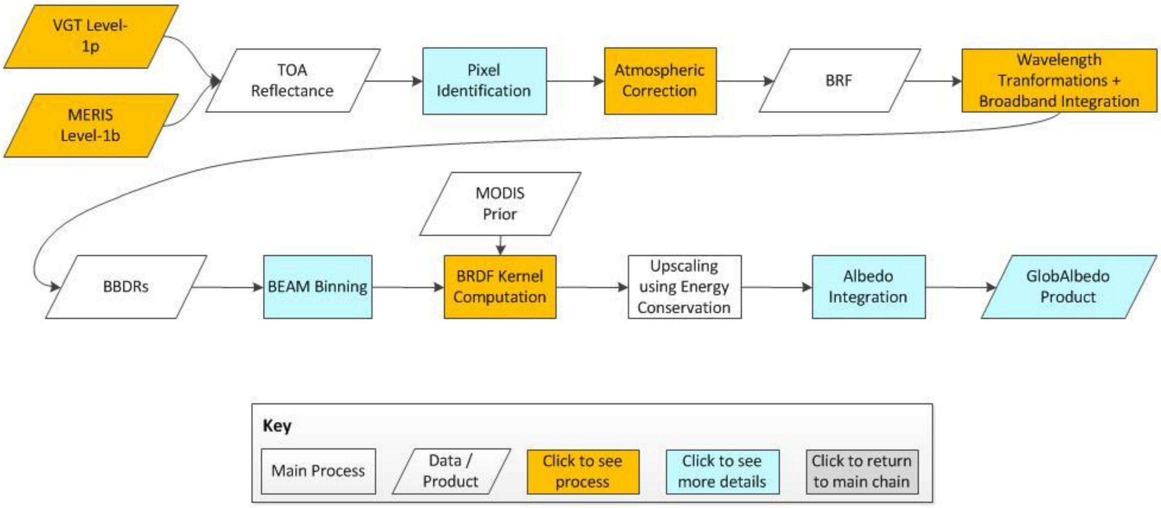

Figure 3. Example traceability diagram for the GlobAlbedo ECV product generation arising from QA4ECV.

8.1.3 Metrological Model

The metrological model chains are intended to describe the set of calibrations, or linkages, of a measurement (or of processed data) to a reference standard. The metrological model describes the origins of the input parameters for the processing model such as the origin of the calibration and characterisation coefficients; be those solely laboratory-based, or occasionally / regularly updated in the field. The aim here is to determine what the fundamental reference for the measurement is. In some cases it will be possible to obtain full metrological traceability - that is, an unbroken chain of calibrations back to the International System of Units (SI). In many cases, however, such a complete chain may not be possible. It is important, however, to show what references do exist. The metrological traceability chain could also be documented as a flow diagram with additional information, containing, for example, references to calibration and characterisation results. Dotted arrows can be used where the link is not strong.

The metrological traceability chain is used to estimate the set of uncertainties (both from random and systematic effects) on the outputs. Note that to be a metrological traceability chain, there is a presumption that all processes have been included and have an estimate of an uncertainty. As part of setting up a metrological model, a review of both the physical and processing model must be made to ensure that all processes are included. As to the uncertainties, where possible, evidence for the magnitude and / or probability distribution of the uncertainties must be provided and documented either through measurements or from Monte-Carlo Analysis (MCA). If no measured uncertainty is available for a process then at least an upper limit to its magnitude must be provided with a rationale for its size. Figure 4 shows an example of a metrological model.

The chain is not used to improve understanding of the processes, nor identify sources of uncertainty; these are both covered by the processing and physical model chains. Therefore, the aim of the chain is to purely demonstrate that linkage to a reference standard is achieved.

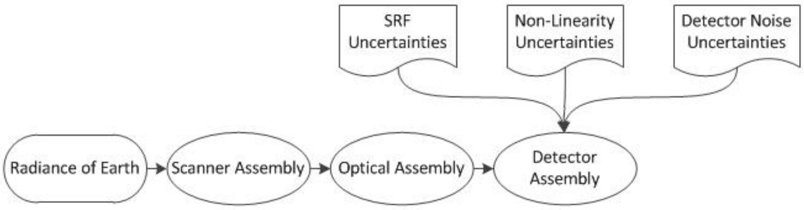

Figure 4. Metrological Chain Example – AVHRR Instrument

8.1.4 Approach to Producing Traceability Chains

- In many cases, the processing model chain is the first type of chain that is produced when describing the traceability of an atmospheric product, as it is the most intuitive type for most users. For many EO satellite applications, the processing model may be the only chain which can realistically be produced in a significant level of detail.

- The physical model involves a more in-depth consideration of the physical processes contributing to the measurement and may be less intuitive for most users.

- The processing and physical model chains are then to be considered iteratively to allow any potential improvements to be made to the processing traceability chain and to ensure that the physical model traceability chain encompasses all relevant elements.

- The metrological model chain should be developed from a combination of the processing and physical models. This chain may have some feedback into the processing and physical model chains; however, this is likely to be limited.

Both the processing and physical model traceability chains will be used for both describing the overall processes associated with an application, as well as being used to describe specific stages. The metrological chain, however, sits alongside the physical & processing chains, and is likely to be used when describing an overall process, rather than the details of individual stages.

The processing, physical and metrological models are then combined to provide an overall model. Alternatively, the overall model can be produced first and split to provide the other models. In either case, it is recognised that producing both the overall model and the set of three other models is not necessary; the production of one or the other is sufficient. **The key aim is ensuring that all relevant data is captured in a systematic manner, whether this be as an overall model, or as three sub-models.** For the technical document deliverable, a single combined chain is required. Figure 5 shows a graphical representation of the sub-model combination. It is noted that the order in which the chains are developed, and the specifics on which each focusses, may vary depending on the application being considered.

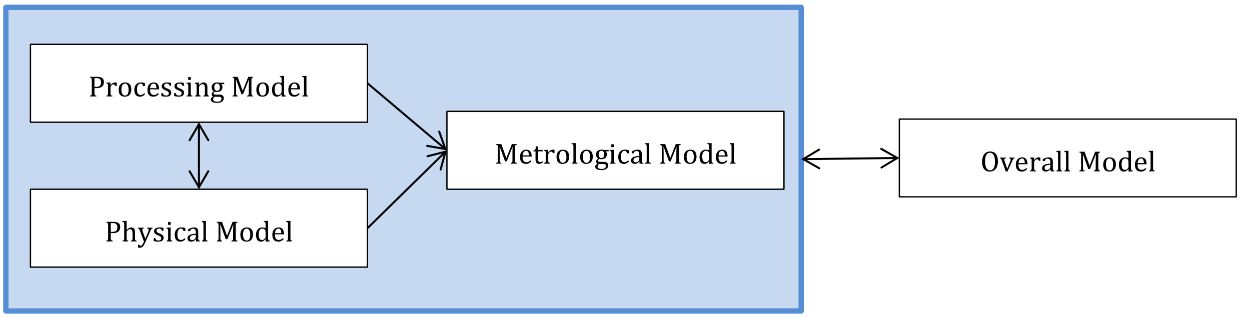

Figure 5: Traceability Chain Production Process

8.2 Representation of the traceability chain

Within the QA4ECV project, a functional prototype of a Traceability and Uncertainty Propagation Tool (TUPT) has been developed[2]. The basic concept of the TUPT is a user-friendly graphical interface that can display (in an electronic interactive format) a visual diagrammatic version of an

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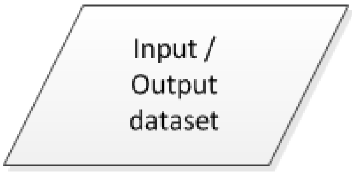
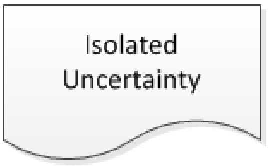
[2] http://qa-system-cgi.com.s3-website.eu-central-1.amazonaws.com/#/

algorithm processing step traceability chain of a product[3]. To provide consistency across QA projects, a similar approach is followed in GAIA CLIM.

The chains should be drawn, graphically, as a series of boxes connected to one another via uni- or bi-directional arrows, as seen in Figure 3.

Table 1. Traceability Chain Shapes and Definitions

	Parallelogram	A dataset visible to the user, be that initial input, final output product or any intermediate product that is available to the user.
	Rectangle	A process within the chain, used to describe a transformation in the dataset that may or may not have an associated uncertainty. The default box shape. The dataflow within the process is typically invisible to the user.
	Rectangle with side-bars	Essential identical to the process rectangle. However, sometimes used to represent a sub-chain or major processing block where more granular information is available.
	Ellipse	Raw data from a measurement device central to the product value or its traceability.
	Rounded rectangle	An ancillary physical quantity dataset or product necessary in the processing chain or to give context to the product.
	Rectangle with wavy bottom	An uncertainty quantity not associated with (isolated from) an element in the traceability chain. Typically used to represent assumptions and known effects that are not directly corrected for.
	Rhombus	A decision step that may affect whether specific data appears in the output product. Such decisions may impact the probability distribution function of the uncertainty.

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[3] http://ec2-52-39-21-246.us-west-2.compute.amazonaws.com/QA4ECV/TCtool.html

Guidance on the types of boxes to be used in GAIA CLIM for each type of chain element is given at Table 1. However, it is noted that the underlying information is the important content, so excessive effort should not be spent in formatting the diagrams. The box type convention follows that used in QA4ECV, but inevitably there will be some variation due to producer choice and the limitations of the software used to create the chain. To date, producers have used MS power point, MS Visio and web-based tools, but the clear display of the information and processes should be paramount, and not limited by formatting concerns.

The colour scheme is not defined, but should be chosen by the producer to best illustrate the commonality in the specific traceability chains. For example, to indicate the raw data sources, the source of traceability, ancillary products, to group a set of boxes which contribute to a single process or, for interactive chains, that further information associated with the box is available.

In developing the guidance, we have created a convention for the traceability identifier numbering as shown in
Figure 6. The 'main chain' from raw measurand to final product forms the axis of the diagram, with top level identifiers (i.e. 1, 2, 3 etc.). Side branch processes add sub-levels components to the top level identifier, (for example, by adding alternate letters & numbers, or 1.3.2 style nomenclature).

The key purpose of this sub-level system is that all the uncertainty from a sub-level are summed in the next level up.

For instance, using
Figure 6, contributors 2a1, 2a2 and 2a3 are all assessed as separate components to the overall traceability chain (have a contribution table). The contribution table for (and uncertainty associated with) 2a, should combine all the sub-level uncertainties (and any additional uncertainty intrinsic to step 2a). In turn, the contribution table for contributor 2, should include all uncertainties in its sub-levels.

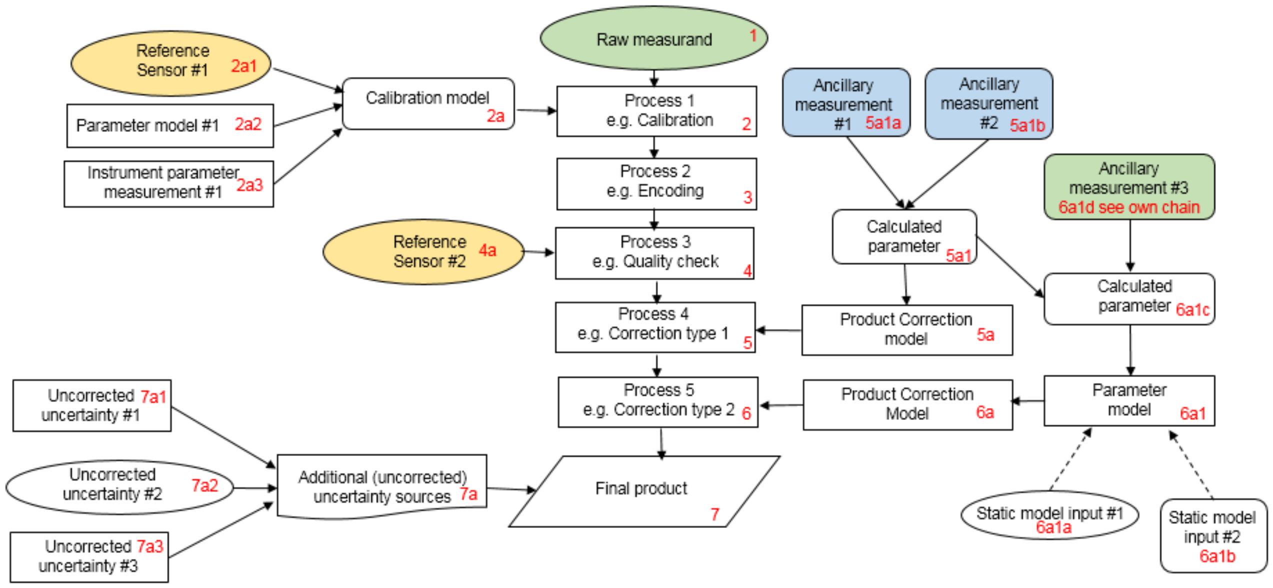


Figure 6. Example traceability chain. Green represents a key measurand or ancillary measurand recorded at the same time with the product raw measurand. Yellow represents a source of traceability. Blue represents a static ancillary measurement

Therefore, only the top level identifiers (1, 2, 3, etc.) in the summary table need be combined to produce the overall product uncertainty. The branches can therefore be considered in isolation, for the more complex traceability chains, with the top level contribution table transferred to the main chain. For instance, see Figure 7 & Figure 8 as an example of how the chain can be divided into a number of diagrams for clearer representation.

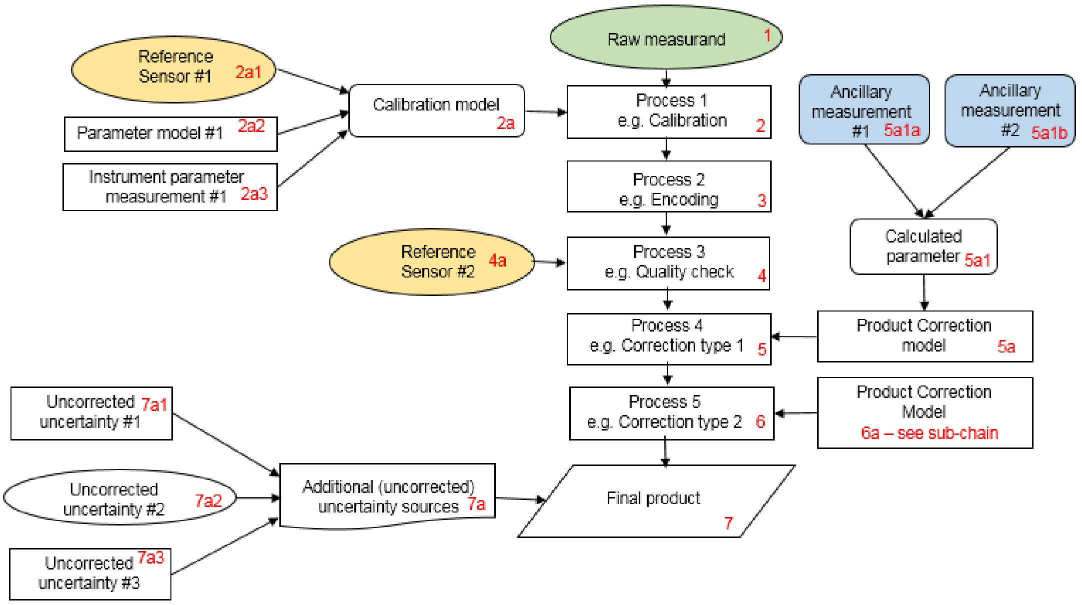


Figure 7. Example chain as sub-divided chain. Green represents a key measurand or ancillary measurand recorded at the same time with the product raw measurand. Yellow represents a source of traceability. Blue represents a static ancillary measurement

When deciding where to create an additional sub-level, the most appropriate points to combine the uncertainties of sub-contributions should be considered, with additional sub-levels used to illustrate there contributions are currently combined in the described process.

A short note on colour coding. Colour coding can/should be used to aid understanding of the key contributors, but we are not suggesting a rigid framework. In Figure 6, green represents a key measurand or ancillary measurand recorded at the same time with the raw measurand; yellow represents a primary source of traceability & blue represents a static ancillary measurement (site location, for instance.) Any colour coding convention you use, should be clearly described.

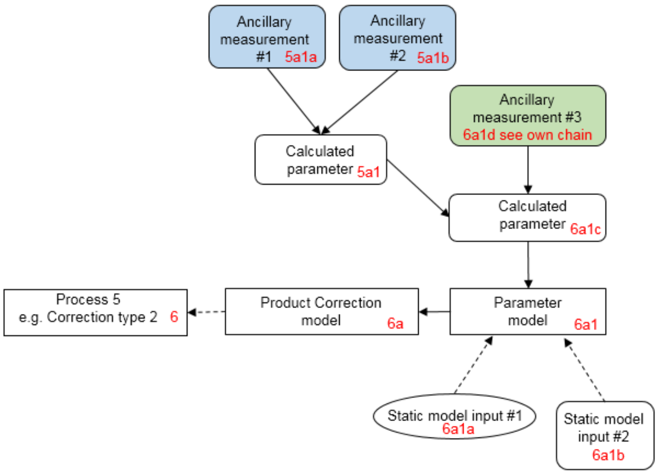


Figure 8. Example chain contribution 6a sub-chain. Green represents a key measurand or ancillary measurand recorded at the same time with the product raw measurand. Blue represents a static ancillary measurement

8.3 Beyond traceability chains

As articulated in the GAIA CLIM Grant Agreement, the vision is to move beyond simple traceability chains (which is effectively understanding the process) towards fiducial reference grade products, encapsulated in a ‘how to measure’ guide and a paper describing the individual produces; for those techniques with sufficient maturity. The ultimate goal is to produce metrologically-rigorous traceable measurements for the target measurement systems, providing practical coverage factors, applicable in the Virtual Observatory (VO). This may not be possible for all the target measurements within the scope of this project, and will depend on the maturity of the contributing partner technique. However, this ultimate goal should be kept in mind.

The full traceability and uncertainty quantification for each instrument type should mirror the process to define the measurement protocols as described in [9]. The analysis algorithm and error characterisation undertaken should result in a technical document describing the measurement procedure, the existing gaps in the uncertainty assessment, and a publication describing the measurement traceability and its uncertainty.

Useful example publications include:

- Documenting the processing chain and corresponding uncertainties [8]
- General information for reference measurements [9]
- Technical instrument report, e.g. [10]
- Deliverable reports from the NORS project [11], specifically the data user guide & uncertainty budget documents.

9 Producing traceability chains for GAIA CLIM

The breadth of techniques and ECVs covered within GAIA CLIM are extensive, so to try to produce a measurement guide & specific descriptive paper covering all possible permutations far extends the scope of the project in terms of available resources. However, in terms of the VO and the GAIA CLIM aim to describe the process in full as a demonstration of the value of such analysis, rigorous end-to-end treatment of a product uncertainty traceability is essential. Consequently, initially the extent of the GAIA CLIM treated measurement product should be clearly defined. For each product a single traceability chain should be developed which captures all the elements of the system including the physical, processing and metrological aspects. Each participant should therefore:

- Identify the exact measurement product to be quantified within GAIA CLIM
  - The specific technique,
  - The specific measurand,
  - The form of the measurand, i.e. profile/total column.
- Identify the specific candidate dataset for the VO.

With a narrowed down scope, it should be possible to:

- Identify the specific elements that make up the product chain for this combination of parameters,
- Identify the inputs, the process, the uncertainties and sensitivities of the element to these parameters.
- Characterise the form of the uncertainty, is it random, quasi-systematic or systematic?
  - Independent random effects e.g. noise

    - Structured random e.g. regular calibration cycles
    - Systematic effects e.g. long term correlation / fixed parameter
- Combine the individual elements and associated uncertainty information to create the overall product chain.

It should be reiterated, that although the approach of considering the physical, processing and metrological models may be helpful in ensuring all parts of the chain/tree have been considered, a single chain should be specified for the specific measurand & technique within GAIA CLIM.

9.1 Practical guidance for GAIA CLIM traceability chains

In characterising the uncertainty, reference to previous work/documentation should be made where relevant, but this should not detract from the independence of the GAIA CLIM measurement document. This document needs to be stand alone, such that it can be understood if read in isolation from the referenced material.

The traceability chains produced should form the basis of this, and require limited additional effort to tailor to the specific case. One concern that should be addressed in the analysis is any differences in site-to-site or user-to-user procedure & observing practice.

- Identify any site-to-site or user-to-user variation in procedure & observing practice from nominally identical instruments so make an assessment of comparability through usage.

The overall measurement equation/chain/tree should consider all contribution factors that feature in the full end-to-end process. This is likely to be sub-divided into branches representative of the major elements within the overall process. Each element should have a summary table of knowledge & traceability including an estimate of contribution magnitude. This assessment may be via:

- a formal analytical treatment
- a sensitivity study
- an educated guess.

Table 2. Shows the summary table to be completed for each process contribution. The notes below add some explanation to the entries.

Information / data	Type / value / equation	Notes / description
Name of effect		
Contribution identifier		
Measurement equation parameter(s) subject to effect		
Contribution subject to effect (final product or sub-tree intermediate product)		
Time correlation extent & form		
Other (non-time) correlation extent & form		

Uncertainty PDF shape		
Uncertainty & units		
Sensitivity coefficient		
Correlation(s) between affected parameters		
Element/step common for all sites/users?		
Traceable to …		
Validation		

Depending on the level of sophistication, the key is to provide a reasonable estimate with the available information. Once the summary table has been completed for the full chain, it should become clear where further work should be focused to most effectively improve the overall level of knowledge of the process uncertainties.

Name of effect – the name of the contribution, should be clear, unique and match the description in the traceability diagram.

Contribution identifier - unique identifier to allow reference in the traceability chains.

Measurement equation parameter(s) subject to effect – The part of the measurement function or equation influenced by this contribution. Ideally, the equation into which the element contributes.

Contribution subject to effect – The top level measurement contribution affected by this contribution. This can be the main product (if on the main chain), or potentially the root of a side branch contribution. It will depend on how the chain has be sub-divided.

Time correlation extent & form – the form & extent of any correlation this contribution has in time.

Other (non-time) correlation extent & form – the form & extent of any correlation this contribution has in a non-time domain. For example, space or spectral.

Uncertainty PDF shape – the probability distribution shape of the contribution, Gaussian/Normal Rectangular, U-shaped, log-normal or other. If the form is not known, a written description is sufficient.

Uncertainty & units – the uncertainty value, including units and confidence interval. This can be a simple equation, but should contain typical values.

Sensitivity coefficient – coefficient multiplied by the uncertainty when applied to the measurement equation.

Correlation(s) between affected parameters – Any correlation between the parameters affected by this specific contribution. If this element links to the main chain by multiple paths within the traceability chain, it should be described here. For instance, SZA or surface pressure may be used separately in a number of models & correction terms that are applied to the product at different points in the processing. See Figure 6, contribution 5a1, for an example.

Element/step common for all sites/users – Is there any site-to-site/user-to-user variation in the application of this contribution?

Traceable to – describe any traceability back towards a primary/community reference.

Validation – Any validation activities that have been performed for this element?

The summary table, explanatory notes and referenced material in the traceability chain should occupy <= 1 page for each element entry.

Once the summary tables have been completed for the full end-to-end process, the uncertainties can be combined, allowing assessment of the combined uncertainty, relative importance of the contributors and correlation scales both temporally & spatially. The unified form of this technical document should then allow easy comparison of techniques and methods.

As described in [9] the establishment of reference level observations consists of definition, execution and evaluation phases. This third phase, the systematic evaluation of the performance of those measurement technologies is partially demonstrated by the metrological evaluation activity here within GAIA CLIM.

9.1.1 Temporal and spatial scales in uncertainty assessment

One elucidating aspect of the uncertainty combination would be to consider correlations on a range of temporal and spatial scales, aligned with different user applications, mirroring the random/systematic levels used to classify the uncertainty contribution form. Considered at the level of:

- Instantaneous measurement (smallest unit of reported data) – potentially dominated by random instrumental effects.
- At the calibration cycle/mid-scale temporal averaging scale – where quasi-systematic instrumental effects are treated as random variables.
- At the longer term temporal or spatial averaged scale for a single site/instrument typified by instrument systematic effects
- At network level, incorporating multiple sites/instruments typified by individual site-specific data treated as random variables.

At these different aggregation scales, different uncertainty contributors will dominate with effects on the magnitude of the overall uncertainty and its probability distribution function form. With the information available from the summary tables, this exercise should not be too onerous, but potentially highlight considerations for user applications other than those primarily of the largely instrumentation-orientated teams working within GAIA CLIM.

9.1.2 Product traceability uncertainty summary

A summary table should follow the individual element assessments, in the form given below. The product traceability uncertainty summary is a summary of the information provided above for this specific product. The purpose of this table is to summarise the assessment and demonstrate at a glance that the dominant contributions to the uncertainty chain have been robustly assessed with adequate traceability.

Element identifier	Contribution name	Uncertainty contribution form	Typical value	Traceability level (L/M/H)	random, structured random, quasi-systematic or systematic?	Correlated to? (Use element identifier)
1						
2						
3						
4						
….						

Table category descriptions.

Element identifier – The name and identifier should correspond to the relevant contributing element in the product traceability uncertainty chain.

Contribution name – the name of the contribution, should be clear, unique and match the description in the traceability diagram.

Uncertainty contribution form - the probability distribution shape of the contribution, Gaussian/Normal Rectangular, U-shaped, log-normal or other.

Typical value – a typical value in the product units.

Traceability level - A description of the traceability associated with this element, following the example set out below.

Traceability Level	Descriptor	Multiplier
High	SI traceable or globally recognised community standard	1
Medium	Developmental community standard or peer-reviewed uncertainty assessment	3
Low	Approximate estimation	10

Although a high level of traceability is desired, this will probably not be the case for all elements. Where that element only makes a small contribution to combined uncertainty, then a lower traceability level would be acceptable. The multiplier values provide one possible mechanism to assess this.

Multiplier value assessment: consider the effect on combined uncertainty of applying multiplier to each particular element. If the combined uncertainty is not significantly increased then the traceability level is adequate for that element. If the combined uncertainty does increase significantly, then further work may be required to improve the traceability level.

Note that the reported uncertainties should not have the multipliers included.

Random, structured random, quasi-systematic or systematic? - A descriptor of the form of the uncertainty.

Correlated to? (Use element identifier) – a descriptor as to whether the element is an independent variable, or has correlations to other elements within the product traceability uncertainty chain.

9.2 Product Traceability Uncertainty document

The output from this work will be a measurement product technical document which should be stand-alone i.e. intelligible in isolation. Reference to external sources (preferably peer-reviewed) and documentation from previous studies is clearly expected and welcomed, but with sufficient explanatory content in the GAIA-CLIM document not to necessitate the reading of all these reference documents to gain a clear understanding of the GAIA-CLIM product and associated uncertainties entered into the VO.

The conclusion to the document should address:

- Typical uncertainties, covering the main modes of operation – e.g. night/day, or any significant altitude dependence.
- Typical uncertainties over a range of time periods/averaging intervals typical of the user community needs.
- Recommendations for improving the uncertainty analysis – e.g. a more detailed assessment of the larger contributors or a first assessment of terms assumed to have negligible contribution.

10 Further reading

Any further study on uncertainty analysis must start with the GUM itself [2]. The GUM is downloadable from http://www.bipm.org/en/publications/guides/gum.html and this website also contains different supplements to the GUM and an introduction to the GUM.

One JCGM supplement that may be of particular interest within GAIA CLIM is ‘Evaluation of measurement data – Supplement 1 to the "Guide to the expression of uncertainty in measurement" – Propagation of distributions using a Monte Carlo method’ JCGM 101:2008 [4]

NPL offers several good practice guides on measurement and uncertainty analysis, with [5] providing a good introduction. NPL also offers a growing range of training courses, e.g. [1] – both face-to-face and e-learning. See:

http://www.npl.co.uk/publications/good-practice-online-modules/.
http://www.npl.co.uk/learning-zone/training/.

The United Kingdom Accreditation Service (UKAS) Publication M 3003, ‘The Expression of Uncertainty and Confidence in Measurement’, http://www.ukas.com/library/Technical-Information/Pubs-Technical-Articles/Pubs-List/M3003_Ed3_final.pdf & Publication EA-4/02 of the European co-operation for Accreditation (EA), ‘Expression of the Uncertainty in Measurement and Calibration’. http://www.european-accreditation.org/publication/ea-4-16-g-rev00-december-2003 may be of interest.

The best introductory textbook to the concepts of the GUM is arguably *“An introduction to uncertainty in measurement” by Les Kirkup and Bob Frenkel*. It is written in a very straightforward way and provides a good overview of the statistical concepts behind the GUM while remaining pragmatic and practical.

A slightly more advanced and detailed, but still very readable book is *“Data reduction and error analysis for the physical sciences” by P.R. Bevington and D.K. Robinson*. This book discusses the statistical basis of uncertainty analysis, and also describes Monte Carlo techniques and least square fitting.

References

[1] Intermediate Uncertainty Analysis for Earth Observation: Instrument Calibration Module, written within the EMRP-funded Metrology for Earth Observation & Climate (MetEOC) project. http://www.emceoc.org/documents/uaeo-int-trg-course.pdf

[2] JCGM, JCGM 100:2008 Evaluation of measurement data – Guide to the expression of uncertainty in measurement, Report, 2008. www.bipm.org/utils/common/documents/jcgm/JCGM_100_2008_E.pdf

[3] JCGM, JCGM 200:2008 International vocabulary of metrology - basic and general concepts and associated terms, Report, 2008. http://www.bipm.org/en/publications/guides/vim.html

[4] JCGM 101:2008 Evaluation of measurement data – Supplement 1 to the "Guide to the expression of uncertainty in measurement" – Propagation of distributions using a Monte Carlo method http://www.bipm.org/utils/common/documents/jcgm/JCGM_101_2008_E.pdf

[5] ‘A Beginner’s Guide to Uncertainty of Measurement’ Measurement Good Practice Guide No. 11 (Issue 2) http://www.npl.co.uk/publications/a-beginners-guide-to-uncertainty-in-measurement

[6] QA4ECV: Gap Analysis of QA4ECV ECV Products D2.2 http://www.qa4ecv.eu/

[7] FIDUCEO project http://www.fiduceo.eu/

[8] Dirksen, R. J., Sommer, M., Immler, F. J., Hurst, D. F., Kivi, R., and Vömel, H.: Reference quality upper-air measurements: GRUAN data processing for the Vaisala RS92 radiosonde, Atmos. Meas. Tech., 7, 4463-4490, doi:10.5194/amt-7-4463-2014, 2014. http://www.atmos-meas-tech.net/7/4463/2014/amt-7-4463-2014.pdf

[9] Immler, F. J., Dykema, J., Gardiner, T., Whiteman, D. N., Thorne, P. W., and Vömel, H.: Reference Quality Upper-Air Measurements: guidance for developing GRUAN data products, Atmos. Meas. Tech., 3, 1217-1231, doi:10.5194/amt-3-1217-2010, 2010. http://www.atmos-meas-tech.net/3/1217/2010/amt-3-1217-2010.html

[10] Report on LIDAR measurements by T. Leblanc. http://tmf.jpl.nasa.gov/tmf-lidar/results/ISSI_Team_Report.htm

[11] NORS (Network Of ground-based Remote Sensing Observations in support of the Copernicus Atmospheric Service) deliverable reports. http://nors.aeronomie.be/index.php/documents

Annex A – Terminology Glossary

In the ‘glossary’ below, a few important words are explained, taken from [5]. Precise or rigorous definitions are not given here. They can be found elsewhere, for example in the *International Vocabulary of Basic and General Terms in Metrology*. A useful and correct set of definitions can also be found in UKAS publication M 3003 *The Expression of Uncertainty and Confidence in Measurement* (See Further Reading in Section 16).

accuracy - closeness of the agreement between a measurement result and true value of that measurand. (Accuracy is a qualitative concept only and is not given a numerical quantity value. It is often misused as uncertainty or precision.)

bias (of a measurement) – estimate of a systematic measurement error

bias (of a measuring instrument) - systematic error of the indication of a measuring instrument

calibration - operation that, under specified conditions, in a first step, establishes a relation between the quantity values with measurement uncertainties provided by measurement standards and corresponding indications with associated measurement uncertainties and, in a second step, uses this information to establish a relation for obtaining a measurement result from an indication. In other words, the comparison of an instrument against a reference or standard, to find any errors in the values indicated by the instrument. In some cases, calibration assigns a relationship between the input and output of an instrument; for example, calibration of a resistance thermometer could relate its output (in ohms) to an input temperature (in degrees Celsius, or in kelvins).

confidence level - number (e.g. 95 %) expressing the degree of confidence in a result

correction (calibration correction) - compensation for an estimated systematic effect. A number added to an instrument reading to correct for an error, offset, or bias. (Similarly, a reading may be multiplied or divided by a ***correction factor*** to correct the value.)

correlation - interdependence, or relationship, between data or measured quantities

coverage factor - number larger than one by which a combined standard measurement uncertainty is multiplied to obtain an expanded measurement uncertainty, for a particular level of confidence

error - measured quantity value minus a reference quantity value. The offset or deviation (either positive or negative) from the correct value

estimated standard deviation - estimate of the standard deviation of the ‘population’ based on a limited sample

expanded uncertainty - product of a combined standard measurement uncertainty and a factor larger than the number one. Standard uncertainty (or combined standard uncertainty) multiplied by a coverage factor k, to give a particular level of confidence

Gaussian distribution - (See ***normal distribution***)

influence quantity - quantity that, in a direct measurement, does not affect the quantity that is actually measured, but affects the relation between the indication and the measurement result; e.g., cloudiness in the field-of-view of an instrument can influence the accuracy of its measurement

interval (confidence interval) - interval containing the set of true quantity values of a measurand with a stated probability, based on the information available. The margin within which the ‘true value’ being measured can be said to lie, with a given level of confidence

level of confidence - number (e.g. 95 %) expressing the degree of confidence in the result

mean (arithmetic mean) - average of a set of numbers

measurand - quantity intended to be measured. The particular quantity subject to measurement

normal distribution - distribution of values in a characteristic pattern of spread (Gaussian curve) with values more likely to fall near the mean than away from it

operator error - a mistake

precision - closeness of agreement between indications or measured quantity values obtained by replicate measurements on the same or similar objects under specified conditions. A term meaning ‘fineness of discrimination’ but often misused to mean ‘accuracy’ or ‘uncertainty’. Its use should be avoided if possible.

random error - component of measurement error that in replicate measurements varies in an unpredictable manner. An error whose effects are observed to vary randomly.

range - absolute value of the difference between the extreme quantity values of a nominal indication. The interval difference between the highest and the lowest of a set of values

reading - value observed and recorded at the time of measurement

rectangular distribution - distribution of values with equal likelihood of falling anywhere within a range

repeatability (of an instrument or of measurement results) - condition of measurement, out of a set of conditions that includes the same measurement procedure, same operators, same measuring system, same operating conditions and same location, and replicate measurements on the same or similar objects over a short period of time. The closeness of the agreement between repeated measurements of the same property under the same conditions.

reproducibility (of an instrument or of measurement results) – condition of measurement, out of a set of conditions that includes different locations, operators, measuring systems, and replicate measurements on the same or similar objects. The closeness of the agreement between measurements of the same property carried out under changed conditions of measurement (e.g. by a different operator or a different method, or at a different time)

resolution - smallest change in a quantity being measured that causes a perceptible change in the corresponding indication. (e.g. a change of one (1) in the last place of a digital display)

result (of a measurement) - set of quantity values being attributed to a measurand together with any other available relevant information. The value obtained from a measurement, either before or after correction or averaging

sensitivity - quotient of the change in an indication of a measuring system and the corresponding change in a value of a quantity being measured. The change in response (of an instrument) divided by the corresponding change in the stimulus

standard deviation - a measure of the spread of a set of results, describing how values typically differ from the average of the set. Where it is not possible to obtain an infinite set of results (in practice it never is) we instead use the estimated standard deviation.

standard uncertainty - measurement uncertainty expressed as a standard deviation.

systematic error – component of measurement error that in replicate measurements remains constant or varies in a predictable manner. A bias or offset (either positive or negative) from the correct value

true value – quantity value consistent with the definition of a quantity, i.e. the value that would be obtained by a perfect measurement

Type A evaluation of uncertainty - evaluation of a component of measurement uncertainty by a statistical analysis of measured quantity values obtained under defined measurement conditions.

Type B evaluation of uncertainty - evaluation of a component of measurement uncertainty determined by means other than a Type A evaluation of measurement uncertainty

uncertainty budget - statement of a measurement uncertainty, of the components of that measurement uncertainty, and of their calculation and combination

uncertainty of measurement - non-negative parameter describing the dispersion of the quantity values being attributed to a measurand. Alternatively described as a quantity representing the doubt in result of a measurement.

uniform distribution - distribution of values with equal likelihood of falling anywhere within a range

validation - the process of assessing, by independent means, the quality of the data products derived from the system outputs

Product Traceability & Uncertainty (PTU) Worked Examples

The annexes contain worked examples of the Product Traceability and Uncertainty documents, written in reference to the guidance given herein.

The GRUAN radiosonde example was developed by NPL as worked examples to be used by the task 2.1.x partners are practical tools to aid in the understanding of the guidance information. Additionally, the GRUAN radiosonde temperature & humidity profiles are regularly used as reference measurements in instrument inter-comparisons, so are a key product dataset for use within GAIA CLIM.

Annex B – GRUAN radiosonde temperature PTU

Annex C – GRUAN radiosonde humidity PTU

Annex D – GRUAN radiosonde geopotential height PTU

Annex E – Microwave radiometer brightness temperature PTU

Annex F – Microwave radiometer temperature profile PTU

Product Traceability and Uncertainty for the GRUAN RS92 radiosonde temperature product

Version 2.0

GAIA-CLIM
Gap Analysis for Integrated
Atmospheric ECV Climate Monitoring
Mar 2015 - Feb 2018

A Horizon 2020 project; Grant agreement: 640276

Date: 30 November 2017

Dissemination level: PU

Work Package 2; Complied by Paul Green &
Tom Gardiner (NPL)

Table of Contents

Version history

Version	Principal updates	Owner	Date
0.1 draft	First draft	NPL	06.02.2017
0.2 draft	Second draft	NPL	18.04.2017
0.3 draft	Third draft	NPL	18.05.2017
0.4 draft	Sent for initial external comments	NPL	24.05.2017
1.0	First issue	NPL	02.06.2017
2.0	Minor changes to chain diagram §5.5 & §5.6 edits. Issued as annex B to D2.6	NPL	30.11.2017

1 Product overview

Product name: In-situ radiosonde RS92 temperature
Product technique: Capacitive temperature sensor
Product measurand: Temperature
Product form/range: profile (ground to 30km, 1sec sampling)
Product dataset: GRUAN Reference level sonde dataset
Site/Sites/Network location:

SITE	LAT	LON	HEIGHT(m)	LOCATION	COUNTRY
BEL	39.05	-76.88	53	Beltsville	US
BOU	71.32	-156.61	8	Boulder	US
CAB	51.97	4.92	1	Cabauw	NL
LAU	-45.05	169.68	370	Lauder	NZ
LIN	52.21	14.12	98	Lindenberg	DE
NYA	78.92	11.92	5	Ny-Ålesund	NO
PAY	46.81	6.95	491	Payerne	CH
POT	40.60	15.72	720	Potenza	IT
SOD	67.37	26.63	179	Sodankylä	FI

Product time period: 20 May 2006 – present
Data provider: GRUAN
Instrument provider: Site operators, see www.gruan.org
Product assessor: Paul Green, NPL
Assessor contact email: paul.green@npl.co.uk

1.1 Guidance notes

For general guidance see the Guide to Uncertainty in Measurement & its Nomenclature, published as part of the GAIA-CLIM project.

This document is a measurement product technical document which should be stand-alone i.e. intelligible in isolation. Reference to external sources (preferably peer-reviewed) and documentation from previous studies is clearly expected and welcomed, but with sufficient explanatory content in the GAIA-CLIM document not to necessitate the reading of all these reference documents to gain a clear understanding of the GAIA-CLIM product and associated uncertainties entered into the Virtual Observatory (VO).

In developing this guidance, we have created a convention for the traceability identifier numbering as shown in Figure 1. The ‘main chain’ from raw measurand to final product forms the axis of the diagram, with top level identifiers (i.e. 1, 2, 3 etc.). Side branch processes add sub-levels components to the top level identifier (for example, by adding alternate letters & numbers, or 1.3.2

style nomenclature).

The key purpose of this sub-level system is that all the uncertainties from a sub-level are summed in the next level up.

For instance, using Figure 1, contributors 2a1, 2a2 and 2a3 are all assessed as separate components to the overall traceability chain (have a contribution table). The contribution table for (and uncertainty associated with) 2a, should combine all the sub-level uncertainties (and any additional uncertainty intrinsic to step 2a). In turn, the contribution table for contributor 2, should include all uncertainties in its sub-levels.

Therefore, only the top level identifiers (1, 2, 3, etc.) shown in bold in the summary table need be combined to produce the overall product uncertainty. The branches can therefore be considered in isolation, for the more complex traceability chains, with the top level contribution table transferred to the main chain. For instance, see Figure 2 & Figure 3 as an example of how the chain can be divided into a number of diagrams for clearer representation.

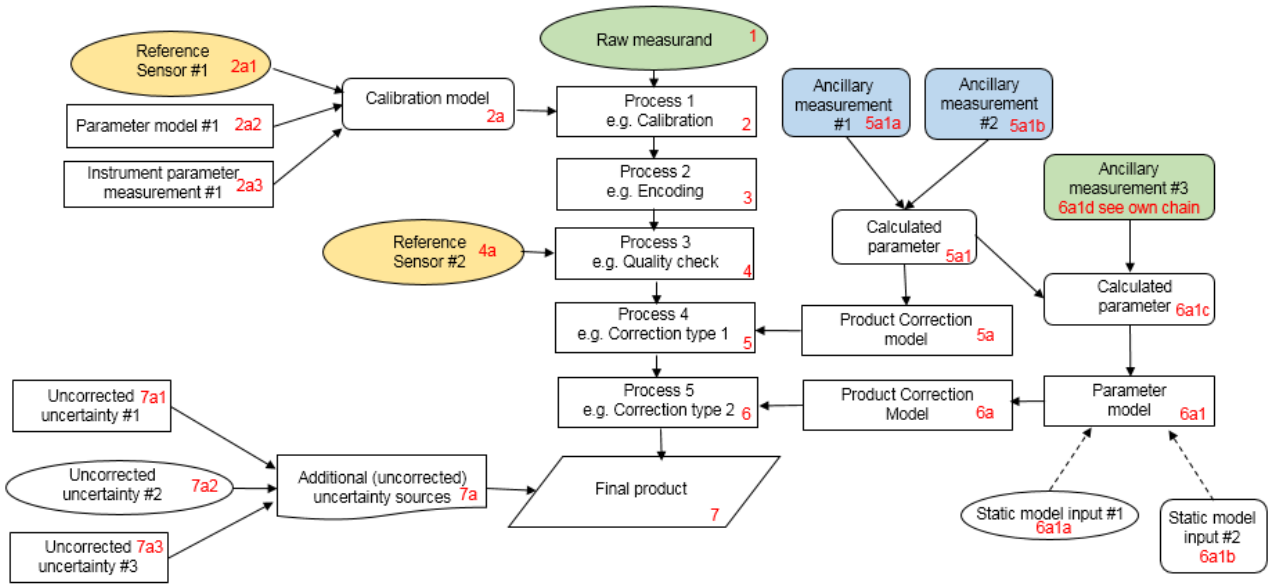


Figure 1. Example traceability chain. Green represents a key measurand or ancillary measurand recorded at the same time with the product raw measurand. Yellow represents a source of traceability. Blue represents a static ancillary measurement

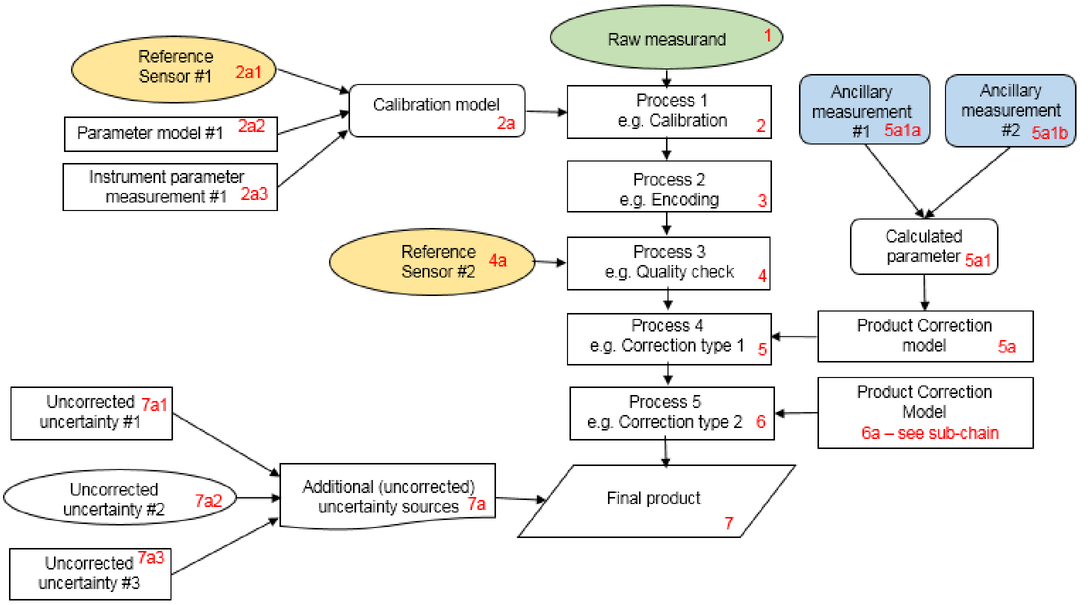


Figure 2. Example chain as sub-divided chain. Green represents a key measurand or ancillary measurand recorded at the same time with the product raw measurand. Yellow represents a source of traceability. Blue represents a static ancillary measurement

When deciding where to create an additional sub-level, the most appropriate points to combine the uncertainties of sub-contributions should be considered, with additional sub-levels used to illustrate where their contributions are currently combined in the described process.

A short note on colour coding. Colour coding can/should be used to aid understanding of the key contributors, but we are not suggesting a rigid framework at this time. In Figure 1, green represents a key measurand or ancillary or complementary measurand recorded at the same time with the raw measurand; yellow represents a primary source of traceability & blue represents a static ancillary measurement (site location, for instance). Any colour coding convention you use, should be clearly described.

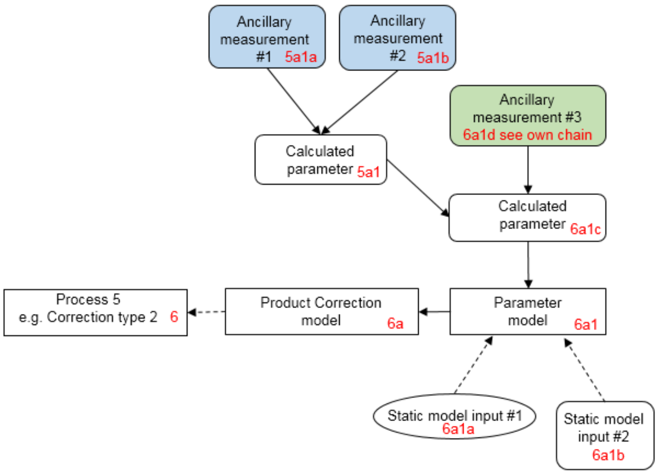


Figure 3. Example chain contribution 6a sub-chain. Green represents a key measurand or ancillary measurand recorded at the same time with the product raw measurand. Blue represents a static ancillary measurement

The contribution table to be filled for each traceability contributor has the form seen in Table 1.

Table 1. The contributor table.

Information / data	Type / value / equation	Notes / description
Name of effect		
Contribution identifier		
Measurement equation parameter(s) subject to effect		
Contribution subject to effect (final product or sub-tree intermediate product)		
Time correlation extent & form		
Other (non-time) correlation extent & form		
Uncertainty PDF shape		
Uncertainty & units		
Sensitivity coefficient		
Correlation(s) between affected parameters		
Element/step common for all sites/users?		
Traceable to …		
Validation		

Name of effect – The name of the contribution. Should be clear, unique and match the description in the traceability diagram.

Contribution identifier - Unique identifier to allow reference in the traceability chains.

Measurement equation parameter(s) subject to effect – The part of the measurement equation influenced by this contribution. Ideally, the equation into which the element contributes.

Contribution subject to effect – The top level measurement contribution affected by this contribution. This can be the main product (if on the main chain), or potentially the root of a side branch contribution. It will depend on how the chain has been sub-divided.

Time correlation extent & form – The form & extent of any correlation this contribution has in time.

Other (non-time) correlation extent & form – The form & extent of any correlation this contribution has in a non-time domain. For example, spatial or spectral.

Uncertainty PDF shape – The probability distribution shape of the contribution, Gaussian/Normal Rectangular, U-shaped, log-normal or other. If the form is not known, a written description is sufficient.

Uncertainty & units – The uncertainty value, including units and confidence interval. This can be a simple equation, but should contain typical values.

Sensitivity coefficient – Coefficient multiplied by the uncertainty when applied to the measurement equation.

Correlation(s) between affected parameters – Any correlation between the parameters affected by this specific contribution. If this element links to the main chain by multiple paths within the traceability chain, it should be described here. For instance, SZA or surface pressure may be used separately in a number of models & correction terms that are applied to the product at different points in the processing. See Figure 1, contribution 5a1, for an example.

Element/step common for all sites/users – Is there any site-to-site/user-to-user variation in the application of this contribution?

Traceable to – Describe any traceability back towards a primary/community reference.

Validation – Any validation activities that have been performed for this element?

The summary table, explanatory notes and referenced material in the traceability chain should occupy <= 1 page for each element entry. Once the summary tables have been completed for the full end-to-end process, the uncertainties can be combined, allowing assessment of the combined uncertainty, relative importance of the contributors and correlation scales both temporally and spatially. The unified form of this technical document should then allow easy comparison of techniques and methods.

2 Introduction

This document presents the Product Traceabililty and Uncertainty (PTU) information for the GRUAN RS92 radiosonde temperature product. The aim of this document is to provide supporting information for the users of this product within the GAIA-CLIM VO, and as an example PTU document for the suppliers of other VO data products. The uncertainty and traceability information contained in this document is based on the details given in Dirksen et al[1].

The GCOS (Global Climate Observing System) Reference Upper-Air Network (GRUAN) data processing for the Vaisala RS92 radiosonde was developed to meet the criteria for reference measurements. These criteria stipulate the collection of metadata, the use of well-documented correction algorithms, and estimates of the measurement uncertainty. An important and novel aspect of the GRUAN processing is that the uncertainty estimates are vertically resolved. Dirksen et al[1] describe the algorithms that are applied in version 2 of the GRUAN processing to correct for systematic errors in radiosonde measurements of pressure, temperature, humidity, and wind, as well as how the uncertainties related to these error sources are derived. Currently, the certified RS92 data product is available from 9 GRUAN sites. An additional GRUAN requirement for performing reference measurements with the RS92 is that the manufacturer- prescribed procedure for the radiosonde’s preparation, i.e. heated reconditioning of the sensors and recalibration during ground check, is followed. In the GRUAN processing however, the recalibration of the humidity sensors that is applied during ground check is removed. For the dominant error source, solar radiation, laboratory experiments were performed to investigate and model its effect on the RS92’s temperature and humidity measurements.

GRUAN uncertainty estimates are 0.15 K for night-time temperature measurements and approximately 0.6 K at 25 km during daytime. The other uncertainty estimates are up to 6 %

relative humidity for humidity, 10–50 m for geopotential height, 0.6 hPa for pressure, 0.4–1 m s^{-1} for wind speed, and 1° for wind direction. Daytime temperature profiles for GRUAN and Vaisala processing are comparable and consistent within the estimated uncertainty. GRUAN daytime humidity profiles are up to 15 % moister than Vaisala processed profiles, of which two-thirds is due to the radiation dry bias correction and one- third is due to an additional calibration correction. Redundant measurements with frost point hygrometers (CFH and NOAA FPH) show that GRUAN-processed RS92 humidity profiles and frost point data agree within 15 % in the troposphere. No systematic biases occur, apart from a 5 % dry bias for GRUAN data around −40 °C at night.

3 Instrument description

The Vaisala RS92 radiosonde, shown in Figure 4, measures vertical profiles of pressure, temperature, and humidity (PTU) from ground to the balloon-burst altitude limit of approximately 40 km. The RS92 is equipped with a wire-like capacitive temperature sensor (“Thermocap”); two polymer capacitive moisture sensors (“Humicap”); a silicon-based pressure sensor; and a GPS receiver to measure position, altitude, and winds. The RS92 transmits sensor data at 1-second intervals, which are received, processed, and stored by the DigiCora ground station equipment. A hydrophobic, reflective coating is applied to the sensor boom and the temperature sensor to reduce the RS92’s sensitivity to solar radiation, and to reduce the deposition of water or ice when flying through clouds. The GPS receiver on the RS92 transmits its position as xyz coordinates in the WGS-84 (World Geodetic System 1984) system. These xyz coordinates are then converted into latitude, longitude, and altitude data by the DigiCora system, while using the readings of the station GPS antenna as a reference for determining the geometric altitude of the radiosonde.

The sensors of the assembled radiosonde are calibrated in Vaisala’s CAL4 calibration facility[2]. The CAL4 contains reference sensors that are recalibrated at regular intervals against standards that are traceable to NIST (for pressure and temperature) and its Finnish equivalent, MIKES (for humidity). The respective operating ranges and accuracies of the PTU sensors are 3 (±0.6) to 1080 (±1) hPa, −90 (±0.5) to 60 (±0.5) ◦C, and 0 (±5) to 100 (±5) % RH, respectively[3].

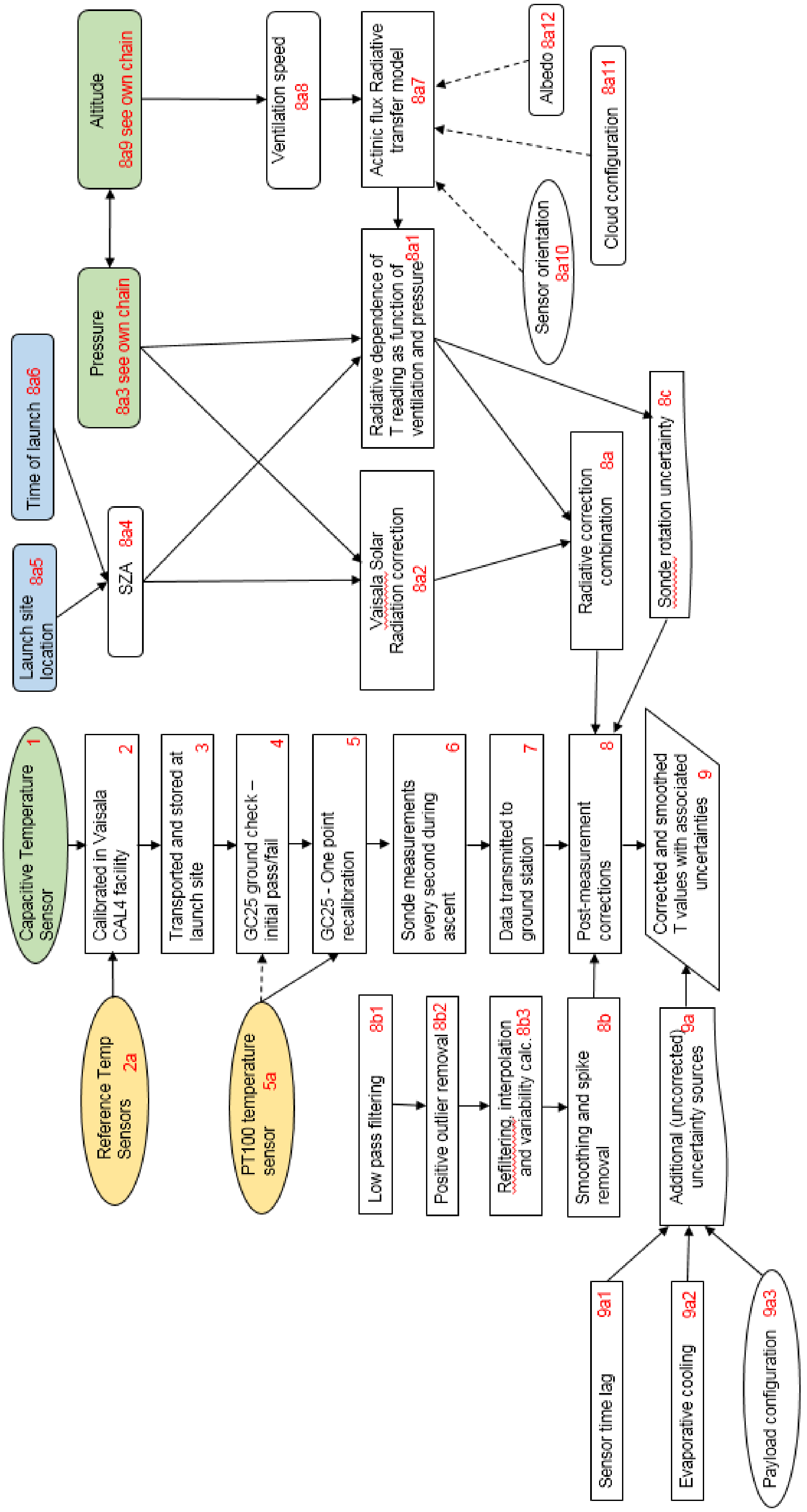
Corrections reduce errors in the temperature and humidity due to solar radiation, time-lag of the RH sensor, and sensor recalibration during the pre-flight ground check. Furthermore, corrections are applied for spurious noise like temperature spikes[4]. Most of these correction algorithms are proprietary and are not disclosed to the user. An overview of relevant modifications in the RS92 hardware and the processing software is available at the Vaisala data continuity website[5]. The RS92 has participated in a number of campaigns and inter-comparisons[6-11]. Campaigns have identified error sources for the RS92 such as radiation dry bias[12] sensor time-lag[13], and a temperature- dependent calibration error for the humidity sensors[12,14].

Figure 4. Photograph of the RS92 radiosonde showing the GPS antenna on the left and the sensor boom on the right. The inset shows the magnified tip of the sensor boom with the wire-shaped temperature sensor and one of the humidity sensors

The temperature sensor of the RS92 radiosonde consists of a temperature-dependent capacitive sensor (Thermocap)[15]. The sensor wire is covered with a reflective, hydrophobic coating to reduce solar heating and systematic errors from evaporative cooling by any water or ice collected during passage through clouds. With an operating range from −90 to +60 ˚C, Vaisala (2007)[4] quotes an accuracy of better than 0.5 K.

The dominant systematic error is due to solar radiative heating. Using a heat transfer model, the radiative error for the RS92 temperature sensor was estimated to be approximately 0.5 K at 35 km[16]. This number is comparable to the correction of up to 0.63 K at 5 hPa that was applied by the DigiCora software (prior to version 3.64) in the processing of RS92 routine soundings until 2010, when this was increased to 0.78 K[5]. The 8th World Meteorological Organization (WMO) radiosonde intercomparison in Yangjiang, China, indicates that the Vaisala-corrected temperature measurements of the RS92 may exhibit a warm bias of up to 0.2 K[8]. A recent comparison between radiosoundings and space- borne GPS radio occultation measurements reports a 0.5–1 K warm bias at 17 hPa for Vaisala-corrected RS92 temperature profiles[17]. The stated accuracy of the satellite-retrieved temperature is approximately 0.2–0.3 K in the middle stratosphere[18,19].

4 Product Traceability Chain



5 Element contributions

5.1 Capacitive Temperature Sensor (1), $u_{u(T)}$

The temperature sensor of the RS92 radiosonde consists of a temperature-dependent capacitive sensor (Thermocap)[20]. The sensor wire is covered with a reflective, hydrophobic coating to reduce solar heating and systematic errors from evaporative cooling by any water or ice collected during passage through clouds. With an operating range from -90 to +60 ◦C, Vaisala[3] quote an accuracy of better than ±0.5 K.

The reported uncertainty associated with the sensor is its statistical uncertainty, defined from the standard deviation, reported in the datafile. Typical values are 0.1-0.15 K (1σ) in the troposphere, rising to 0.5 K (1σ) at 10 hPa.

Information / data	Type / value / equation	Notes / description
Name of effect	Capacitive temperature sensor	
Contribution identifier	1, statistical uncertainty $u_{u(T)}$	
Measurement equation parameter(s) subject to effect	Temperature	
Contribution subject to effect (final product or sub-tree intermediate product)	Temperature	
Time correlation extent & form	None	Random over ascent
Other (non-time) correlation extent & form	None	Random over ascent
Uncertainty PDF shape	Normal	
Uncertainty & units	±0.5 K (2σ) [accuracy] & 0.1-0.15 K (1σ) in the trop., rising to 0.5 K (1σ) at 10 hPa [statistical unc.]	
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	Accuracy to 2	Calibration in Vaisala CAL4 facility
Validation	Inter-comparison studies.	

5.2 Calibration in Vaisala CAL4 facility (2) $u_{c, cal(T)}$

Radiosonde sensor calibration curves determined in Vaisala CAL4 facility over a range of temperatures and pressures.

Information / data	Type / value / equation	Notes / description
Name of effect	Vaisala CAL4 facility calibration	
Contribution identifier	2, $u_{c, cal(T)}$	
Measurement equation parameter(s) subject to effect	Temperature	
Contribution subject to effect (final product or sub-tree intermediate product)	Temperature	
Time correlation extent & form	None	Assuming that each sensor is calibrated independently. If not then there may be correlation across batches.
Other (non-time) correlation extent & form	None	See above
Uncertainty PDF shape	Normal	Assumed
Uncertainty & units (1σ)	±0.15 K (1σ)	Repeatability of calibration
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	2a - reference T sensor	
Validation	Inter-comparison studies.	

5.3 Reference T Sensors (2a)

The CAL4 contains PTU reference sensors that are recalibrated at regular intervals against standards that are traceable to NIST (for pressure and temperature) and its Finnish equivalent, MIKES (for humidity). The respective operating ranges and accuracies of the PTU sensors are 3 (±0.6) to 1080 (±1) hPa,−90 (±0.5) to 60 (±0.5) ˚C, and 0 (±5) to 100 (±5) % RH, respectively[3].

Information / data	Type / value / equation	Notes / description
Name of effect	Reference T sensors	Reference sensors in Vaisala CAL4 facility
Contribution identifier	2a	
Measurement equation parameter(s) subject to effect	Temperature	
Contribution subject to effect (final product or sub-tree intermediate product)	CAL4 calibration	
Time correlation extent & form	Long-term	Correlated over period of reference sensor recalibration.
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	<±0.1 K (2σ)	Assumed to be at least as good as GC25 reference sensor.
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	NIST	Temperature and pressure
Validation	Intercomparison studies	Indirect validation

5.4 Transported and stored at launch site (3)

Radiosondes are shipped from Vaisala to launch location and then stored on site. It is currently assumed that any changes to sensor performance during this period is corrected for by the Ground Check.

Information / data	Type / value / equation	Notes / description
Name of effect	Transportation and storage	
Contribution identifier	3	
Measurement equation parameter(s) subject to effect	Temperature	
Contribution subject to effect (final product or sub-tree intermediate product)	Temperature	

Time correlation extent & form	None	Assuming no batch dependence.
Other (non-time) correlation extent & form	None	Assuming no batch dependence.
Uncertainty PDF shape	N/A	
Uncertainty & units (1σ)	0	Assumes that effect corrected by Ground Check
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	N/A	
Validation	N/A	

5.5 GC25 ground check – initial pass/fail (4)

The manufacturer's operational procedure demands that prior to flight a ground check is performed. During this check the sensor boom is inserted into a calibration unit (GC25) and the sensors are heated to remove contaminants that introduce a dry bias in the humidity measurements ("reconditioning"). The initial quality control verifies that the readings of the PTU sensors during the ground check are within pre-defined limits before GRUAN corrections are applied. For the data to be processed, the corrections determined inthe GC25 must be less than 1K for T, 1.5 hPa for P, and less than 2% RH for U.

Information / data	Type / value / equation	Notes / description
Name of effect	GC25 Pass/Fail	
Contribution identifier	4	
Measurement equation parameter(s) subject to effect	Temperature	
Contribution subject to effect (final product or sub-tree intermediate product)	Temprerature	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Rectangular	
Uncertainty & units (1σ)	<1K* Typically ±0.3 K (2σ)	Not a formal uncertainty value. Cut-off to ensure no sensors with >1K difference are flown.

Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	GC25 T sensor	
Validation	N/A	

5.6 GC25 - One point recalibration (5) u_{GC25}

The manufacturer’s operational procedure demands that prior to flight a ground check is performed. During this check the sensor boom is inserted into a calibration unit (GC25) and the sensors are heated to remove contaminants that introduce a dry bias in the humidity measurements (“reconditioning”). A one-point recalibration is applied to the PTU, based on comparing the temperature and pressure sensors to a PT100 temperature sensor and the station barometer, respectively, and recording the humidity sensor readings in a dry zone over a bed of desiccant.

The uncertainty components of GC25 temperature measurement are the calibration uncertainty, the long-term stability of the Pt-100, the reference resistor and the GC25 electronics uncertainty (A/D transformation etc.).

Combined uncertainty: ± 0,098°C 2-sigma (k=2) confidence level (95.5%). For long-term stability a maximum value of 0.05 °C is assumed.

The uncertainty in this step would be a combination of the GC25 measurement uncertainty and the GC25 ground check difference, so typically $\sqrt{[((\pm 0.1\text{ K})^2 + ((\pm 0.4\text{ K})/3)^2]} = \pm 0.17$ K

Information / data	Type / value / equation	Notes / description
Name of effect	GC25 recalibration	Not known if shift or scale adjustment
Contribution identifier	5, u_{GC25}	
Measurement equation parameter(s) subject to effect	Temperature	
Contribution subject to effect (final product or sub-tree intermediate product)	Temperature	
Time correlation extent & form	Systematic over flight	
Other (non-time) correlation extent & form	Systematic over flight	
Uncertainty PDF shape	Rectangular	Difference during ground check
Uncertainty & units (2σ)	$\sqrt{u_c^2 + (\frac{\Delta T_{GC25}}{3})^2}$	Combined with Vaisala calibration uncertainty

	typically 0.17 K (2σ)	
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	PT100 (5a)	
Validation	Intercomparisons	Indirect

5.7 PT100 temperature sensor (5a)

Ground-check calibration unit (GC25) contains a PT100 Platinum Resistance Temperature Detector as the temperature reference.

Information / data	Type / value / equation	Notes / description
Name of effect	PT100 temperature sensor	
Contribution identifier	5a	
Measurement equation parameter(s) subject to effect	Temperature	
Contribution subject to effect (final product or sub-tree intermediate product)	GC25 recalibration	
Time correlation extent & form	Long-term systematic	Systematic between PT100 replacement
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	Assumed
Uncertainty & units (1σ)	±0.15 K	Assumes a Class A resistance tolerance: ±(0.15 + 0.002*t)°C or 100.00 ±0.06 O at 0ºC
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	PT100 specifications	Assuming the PT100 is not calibrated against a reference standard
Validation	N/A	

5.8 Sonde measurements every second during ascent (6)

A radiosonde temperature measurement is recorded every second during the sonde ascent. The uncorrelated uncertainty of these measurements (measurement noise) is assessed as part of the spike removal algorithm (Contribution 8b) within the post-measurement corrections (Contribution 8). It is assumed there are no other uncertainty sources within this step.

Information / data	Type / value / equation	Notes / description
Name of effect	Temperature measurments during sonde ascent	
Contribution identifier	6	
Measurement equation parameter(s) subject to effect	Temperature	
Contribution subject to effect (final product or sub-tree intermediate product)	Temperature	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	N/A	
Uncertainty & units (1σ)	None	Covered in spike removal algorithm (8b)
Sensitivity coefficient	1	
Correlation(s) between affected parameters	1	
Element/step common for all sites/users?	Yes	
Traceable to …	N/A	
Validation	Intercomparisons	

5.9 Data transmitted to ground station (7)

It is assumed there are no issues/uncertainties associated with data transmission from the radiosonde to the ground station.

Information / data	Type / value / equation	Notes / description
Name of effect	Data transmission	
Contribution identifier	7	
Measurement equation parameter(s) subject to effect	Temperature	

Contribution subject to effect (final product or sub-tree intermediate product)	Temperature	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	N/A	
Uncertainty & units (1σ)	0	
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	N/A	
Validation	N/A	

5.10 Post-measurement corrections (8)

The dominant systematic error is due to solar radiative heating (radiative correction (8a)). Smoothing & spike removal (8b) is the other post-measurment correction.

This contribution is the combined effect of all these corrections.

Information / data	Type / value / equation	Notes / description
Name of effect	Post-measurement correction	Combined 8a & 8b
Contribution identifier	8	
Measurement equation parameter(s) subject to effect	$T' = T - \Delta T$	
Contribution subject to effect (final product or sub-tree intermediate product)	Temperature	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	±0.22 K (2σ) in trop. ±0.5 K (2σ) in strat.	Combination of branch 8 sub-elements.
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	

Element/step common for all sites/users?	Yes	
Traceable to …		
Validation		

5.11 **Radiative correction (8a)**

The mean of the GRUAN and Vaisala radiative corrections is used for the daytime measurements. Only the Vaisala correction is used for nighttime measurments.

The GRUAN radiation correction, relies on laboratory experiments and radiative transfer calculations to estimate the actinic flux on the sensor. Laboratory work has determined the relation between temperature error and actinic flux as a function of pressure and ventilation.
Other sources of error include temperature spikes[4] due to patches of warm air coming off the sensor housing and the balloon, evaporative cooling of the wetted sensor after exiting a cloud and sensor time-lag. The last two effects are not corrected because no appropriate correction algorithm is available for evaporative cooling, although affected data points should be flagged and the impact of time-lag is considered negligible.

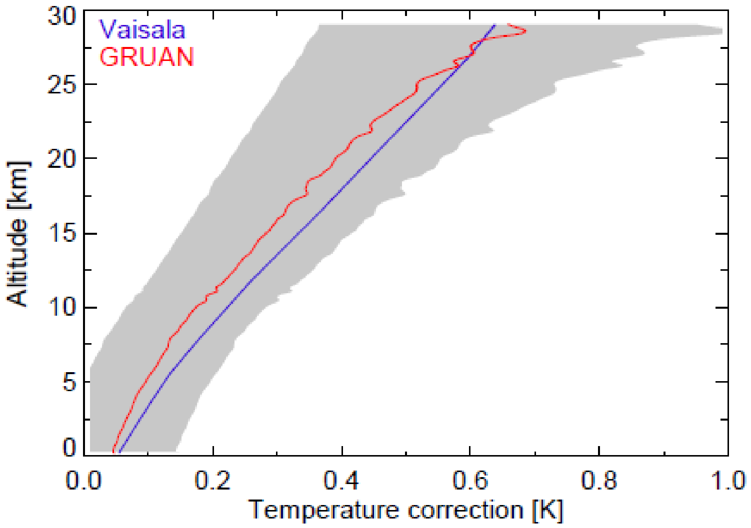


Figure 7. Comparison of the GRUAN and Vaisala correction models for the radiation temperature error. Blue trace: Vaisala correction profile (DigiCora version 3.64); red trace: GRUAN correction profile. The grey bar represents the uncertainty estimate of the GRUAN temperature correction. The correction profiles are evaluated for a sounding performed at Lindenberg on 17 September 2013 at 12:00 UTC; maximum solar zenith angle during the sounding: 36.5°.

Figure 5. Dirksen et al[1] figure 7, showing typical corrections for the solar radiation effects on temperature.

Information / data	Type / value / equation	Notes / description
Name of effect	Radiative correction	Combined of GRUAN and Vaisala corrections
Contribution identifier	8	
Measurement equation parameter(s) subject to effect	$T' = T + (\Delta T_G + \Delta T_V)/2$	During daytime. $T' = T + \Delta T_V$, at night.
Contribution subject to effect (final product or sub-tree intermediate product)	Temperature	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	<0.36 K (2σ)	Combination of the 8a sub-elements
Sensitivity coefficient	1	
Correlation(s) between affected parameters	none	
Element/step common for all sites/users?	yes	
Traceable to …		
Validation		

5.12 Radiative dependence of T reading as function of ventilation and pressure (8a1) $u_{c,RC(\Delta T)}$

During daytime the radiosonde sensor boom is heated by solar radiation, which introduces biases in temperature and humidity. The net heating of the temperature sensor depends on the amount of absorbed radiation and on the cooling by thermal emission and ventilation by air flowing around the sensor. Luers[22] used customized radiative transfer calculations and detailed information on the actual cloud configuration to accurately compute the radiation temperature error for selected soundings.

$$\Delta T(I_a, p, v) = a \cdot x^b \qquad \text{with } x = \frac{I_a}{p \cdot v},$$

a = 0:18 ± 0.03 and b = 0:55 ± 0:06, the uncertainty due to these parameters in a, b and the radiation correction is typically <0.2 K (2σ) daytime only. For nightime the Vaisala correction of 0.04 K at 5 hPa is used.

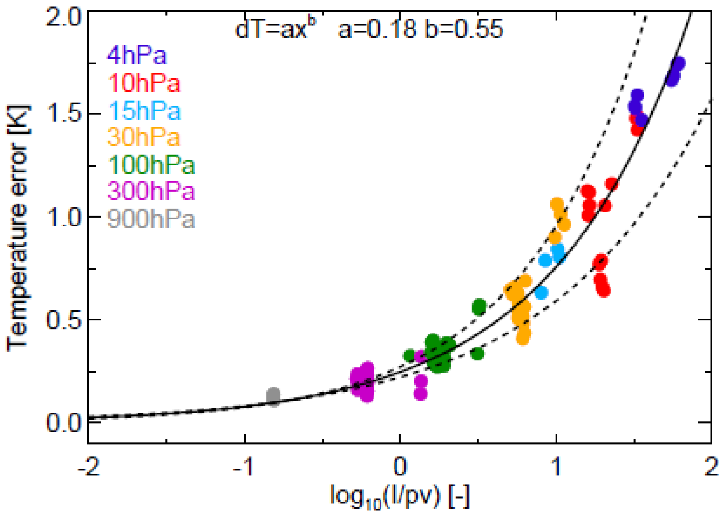


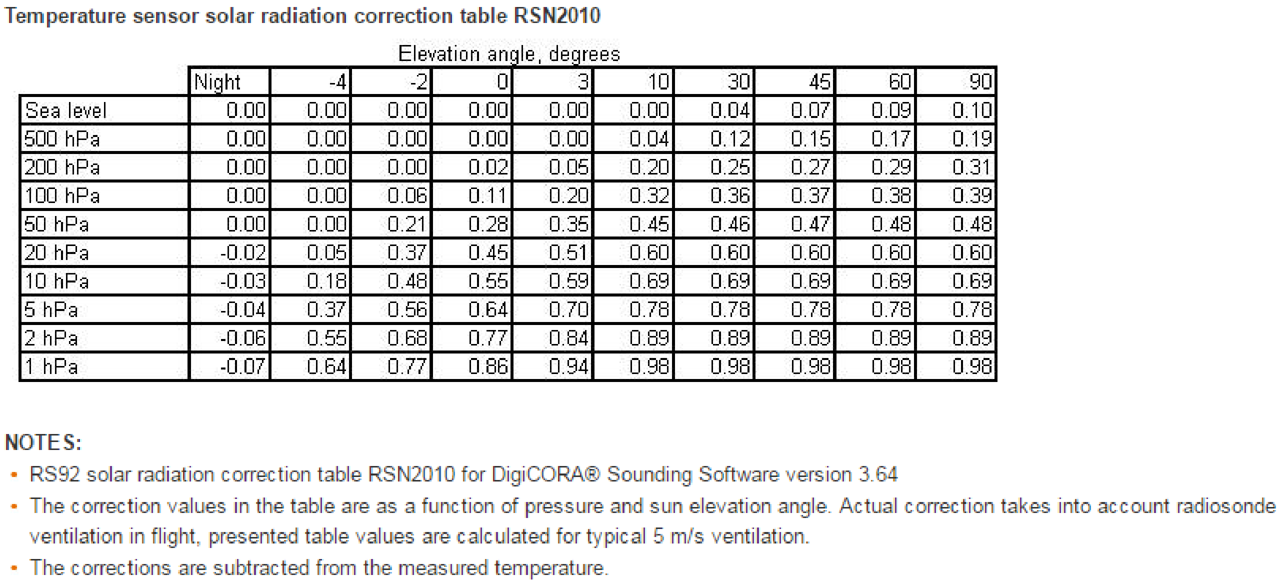
Figure 6. Dirksen et al[1] figure 4

Information / data	Type / value / equation	Notes / description
Name of effect	Radiative dependence of T f(ventilation, pressure)	
Contribution identifier	8a1, $u_{c,RC(\Delta T)}$	
Measurement equation parameter(s) subject to effect	$T' = T - \Delta T,$ $where\ \Delta T = a.\left(\frac{I_a}{p.v}\right)^b$	
Contribution subject to effect (final product or sub-tree intermediate product)	Radiation correction	
Time correlation extent & form	None	Point to point correction
Other (non-time) correlation extent & form	N/A	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)		
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …		
Validation		

5.13 **Vaisala radiation correction (8a2)**

The Vaisala correction for the radiation temperature error is available as a table for various pressures and solar elevation angles[23]. The ascent speed is assumed to be 5 m/s, so does not use the measured values.

There is no separate uncertainty associated with the DigiCora correction in Dirksen et al[1]. However, validation experiments shows a standard deviation of 0.1 K in the troposphere, rising to between 0.3 K and 0.4 K in the stratosphere.



Temperature sensor solar radiation correction table RSN2010

	Elevation angle, degrees									
	Night	-4	-2	0	3	10	30	45	60	90
Sea level	0.00	0.00	0.00	0.00	0.00	0.00	0.04	0.07	0.09	0.10
500 hPa	0.00	0.00	0.00	0.00	0.00	0.04	0.12	0.15	0.17	0.19
200 hPa	0.00	0.00	0.00	0.02	0.05	0.20	0.25	0.27	0.29	0.31
100 hPa	0.00	0.00	0.06	0.11	0.20	0.32	0.36	0.37	0.38	0.39
50 hPa	0.00	0.00	0.21	0.28	0.35	0.45	0.46	0.47	0.48	0.48
20 hPa	-0.02	0.05	0.37	0.45	0.51	0.60	0.60	0.60	0.60	0.60
10 hPa	-0.03	0.18	0.48	0.55	0.59	0.69	0.69	0.69	0.69	0.69
5 hPa	-0.04	0.37	0.56	0.64	0.70	0.78	0.78	0.78	0.78	0.78
2 hPa	-0.06	0.55	0.68	0.77	0.84	0.89	0.89	0.89	0.89	0.89
1 hPa	-0.07	0.64	0.77	0.86	0.94	0.98	0.98	0.98	0.98	0.98

NOTES:

- RS92 solar radiation correction table RSN2010 for DigiCORA® Sounding Software version 3.64
- The correction values in the table are as a function of pressure and sun elevation angle. Actual correction takes into account radiosonde ventilation in flight, presented table values are calculated for typical 5 m/s ventilation.
- The corrections are subtracted from the measured temperature.

Figure 7. DigiCora radiation correction table[24]

Information / data	**Type / value / equation**	**Notes / description**
Name of effect	Vaisala radiation correction	
Contribution identifier	8a2	
Measurement equation parameter(s) subject to effect	T’ = T - ΔT	
Contribution subject to effect (final product or sub-tree intermediate product)	Temperturature	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	0.1 K in the troposphere, up to 0.4 K in the stratosphere.	Derived from validation experiments but not included in overall uncertainty assessment.
Sensitivity coefficient	1	

Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …		
Validation	Vaisala validation experiments	

5.14 Pressure (8a3)

The pressure derived from the GRUAN sonde pressure measurement is used in both the GRUAN and Vaisala solar radiation correction models.

The quoted pressure uncertainty is ±0.2 hPa (1σ). When applied to the GRUAN solar correction model the typical temperature uncertainties are <0.001 K (1σ) in the troposphere, rising to ±0.03 K (1σ) in the stratosphere. See the GRUAN pressure product traceability uncertainty document for details of this uncertainty contribution.

Information / data	Type / value / equation	Notes / description
Name of effect	Pressure	
Contribution identifier	8a3	
Measurement equation parameter(s) subject to effect	Input into both solar radiation correction models	For the GRUAN correction takes form $\Delta T(I_a, p, v) = a \cdot x^b \quad \text{with } x = \frac{I_a}{p \cdot v},$
Contribution subject to effect (final product or sub-tree intermediate product)	Solar radiation correction	
Time correlation extent & form	Systematic over part of ascent	
Other (non-time) correlation extent & form	Systematic over part of ascent	
Uncertainty PDF shape	Normal & offset	
Uncertainty & units	±0.2 hPa (1σ), typically <0.001 K (1σ) in the troposphere, rising to ±0.03 K (1σ) in the strat.	For the GRUAN solar radiation correction.
Sensitivity coefficient	1	
Correlation(s) between affected parameters	Altitude	
Element/step common for all sites/users?	Yes	
Traceable to …		

Validation		

5.15 Solar Zenith Angle (8a4)

The uncertainty is not considered separately, but is effectively incorporated into the 8a2 Actinic flux radiative transfer model fit uncertainty.

Information / data	Type / value / equation	Notes / description
Name of effect	Solar Zenith Angle	
Contribution identifier	8a4	
Measurement equation parameter(s) subject to effect	-	
Contribution subject to effect (final product or sub-tree intermediate product)	Actinic flux radiative transfer model	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Static	
Uncertainty & units (1σ)	0	
Sensitivity coefficient	1	
Correlation(s) between affected parameters		
Element/step common for all sites/users?		
Traceable to …		
Validation		

5.16 Launch site location (8a5)

The uncertainty is not considered separately.

Information / data	Type / value / equation	Notes / description
Name of effect	Launch site location	
Contribution identifier	8a5	
Measurement equation parameter(s) subject to effect	-	

Contribution subject to effect (final product or sub-tree intermediate product)	SZA	Uses site longitude/latitude & altitude
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Static	
Uncertainty & units (1σ)	0	
Sensitivity coefficient	1	
Correlation(s) between affected parameters		
Element/step common for all sites/users?		
Traceable to …		
Validation		

5.17 Time of launch (8a6)

The uncertainty is not considered separately.

Information / data	Type / value / equation	Notes / description
Name of effect	Time of launch	
Contribution identifier	8a6	
Measurement equation parameter(s) subject to effect	-	
Contribution subject to effect (final product or sub-tree intermediate product)	SZA	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Static	
Uncertainty & units (1σ)	0	
Sensitivity coefficient	1	
Correlation(s) between affected parameters		
Element/step common for all sites/users?		
Traceable to …		

Validation		

5.18 Actinic flux radiative transfer model (8a7)

The dominant systematic error is due to solar radiative heating. Using a heat transfer model, the radiative error for the RS92 temperature sensor was estimated to be approximately 0.5 K at 35 km[16]. This number is comparable to the correction of up to 0.63 K at 5 hPa that was applied by the DigiCora software (prior to version 3.64) in the processing of RS92 routine soundings until 2010, when this was increased to 0.78 K[5].

The 8th World Meteorological Organization (WMO) radiosonde intercomparison in Yangjiang, China, indicates that the Vaisala-corrected temperature measurements of the RS92 may exhibit a warm bias of up to 0.2 K[8].

A recent comparison between radiosoundings and spaceborne GPS radio occultation measurements reports a 0.5–1K warm bias at 17 hPa for Vaisala-corrected RS92 temperature profiles[17]. The reported accuracy of the satellite-retrieved temperature is approximately 0.2–0.3K in the middle stratosphere[18,19].

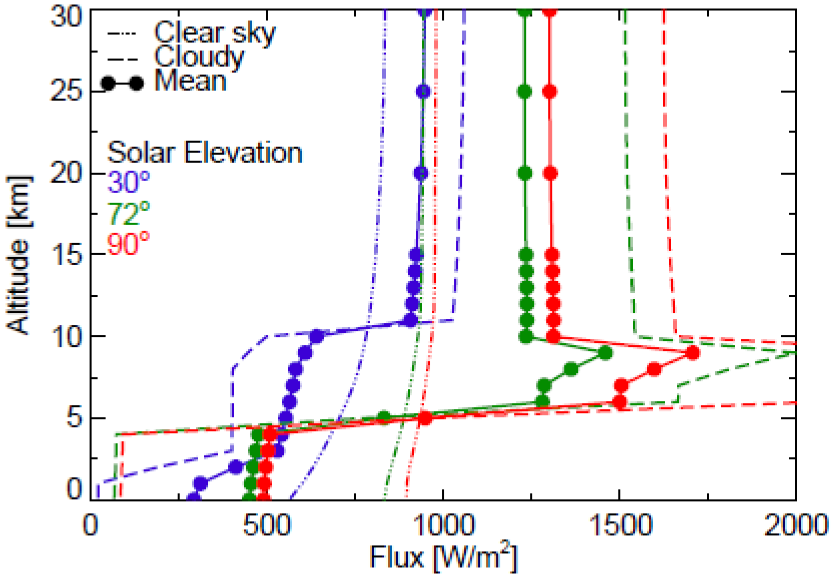


Figure 8. Dirksen figure 5

Information / data	Type / value / equation	Notes / description
Name of effect	Actinic flux model	
Contribution identifier	8a7	
Measurement equation parameter(s) subject to effect	Radiation correction temperature correction $\Delta T = a.\left(\frac{I_a}{p.v}\right)^b$	

Contribution subject to effect (final product or sub-tree intermediate product)	Radiation correction	
Time correlation extent & form	Corrected point by point. correlates with time of day (SZA)	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Rectangular	
Uncertainty & units (1σ)	60-250 W/m^2 in the troposphere, 30-200 W/m^2 in the stratosphere dependant on SZA	$u(I_\mathrm{a}) = \frac{\lvert I_{\mathrm{a,\,cloudy}} - I_{\mathrm{a,\,clear\ sky}} \rvert}{2\sqrt{3}}.$ Low end of range at low SZA, high end of range at high SZA
Sensitivity coefficient	$\Delta T \sim {I_a}^b$	
Correlation(s) between affected parameters	SZA	
Element/step common for all sites/users?	Yes	
Traceable to …		
Validation		

5.19 Ventilation speed (8a8) u_v & $u_{vent(\Delta T)}$

The correction of the radiation temperature error also depends on the ventilation speed v. The temperature correction is a function of pressure & ventilation speed, given in Figure 9.

In the GRUAN processing the actual ventilation speed is used, rather than assuming a fixed value. The actual ventilation speed is the sum of the ascent speed, which is derived from the altitude data, plus an additional contribution due to the sonde’s pendulum motion.

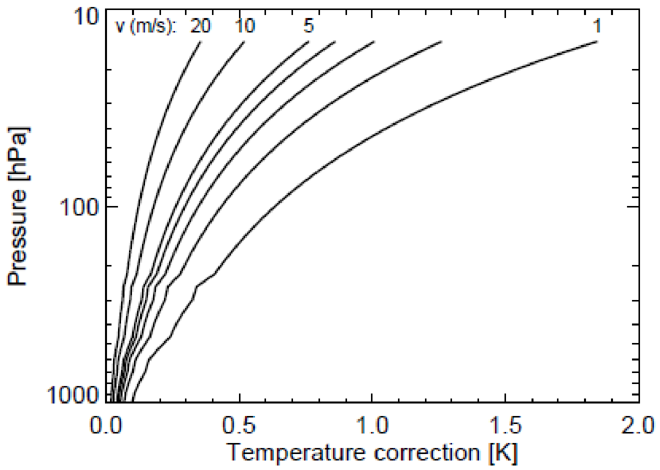


Figure 6. Profiles of the GRUAN radiation temperature correction for ventilation speeds between 1 and 20 $\mathrm{m\,s^{-1}}$. The correction was calculated for a radiosounding performed in Lindenberg on 17 September 2013 at 12:00 UTC. The kinks in the profiles between 900 and 200 hPa result from the cloud configuration that was used in the Streamer simulations, with cloud layers between 4 and 6 and between 7 and 10 km, which introduces jumps in the simulated radiation profile at the top of the cloud (see the dashed traces in Fig. 5). The maximum solar zenith angle during the sounding was 36.5°.

Figure 9. Ventilation speed temperature correction, from Dirksen et al[1] figure 6

$u(v) = \pm 1\,\mathrm{m/s}\ (2\sigma)$, with the temperature dependence given by:

$$\Delta T \cdot u(v)/v$$

This is equivilant to 0.01 K in the troposphere, rising upto 0.3 K in the stratosphere (2σ).

Information / data	Type / value / equation	Notes / description
Name of effect	Ventilation speed correction	
Contribution identifier	8a4, u_v & $u_{vent(\Delta T)}$	
Measurement equation parameter(s) subject to effect	Temperature	
Contribution subject to effect (final product or sub-tree intermediate product)	Radiation correction (8)	$\Delta T \cdot u(v)/v$
Time correlation extent & form	Systematic	Over ascent
Other (non-time) correlation extent & form	Systematic with Altitude measurement and assumed pendulum motion	Correlated to altitude systematic errors.
Uncertainty PDF shape	Rectangular in velocity, but treated as random in ΔT.	Increase in ventilation speed correction is $+1\ \mathrm{m.s^{-1}} \pm 1\mathrm{m.s^{-1}}$ suggesting a defined limit uncertainty.

Uncertainty & units (1σ)	u(v) = ±1m/s (2σ), with the temperature dependence given by $\Delta T \cdot u(v)/v$ Equivilant to 0.01 K (in the trop. upto 0.3 K in the strat (2σ)	
Sensitivity coefficient	1	
Correlation(s) between affected parameters	Altitude measurement	
Element/step common for all sites/users?	Yes	
Traceable to …		
Validation		

5.20 **Altitude (8a9)**

Not considered separately – only uncertainty on derived vertilation speed (8a5).

The altitude product from the GRUAN sondes have a typical uncertainty of ±1 m (1σ) in the troposphere, increasing to ±1.5 m (1σ) in the stratosphere.

Information / data	Type / value / equation	Notes / description
Name of effect	Altitude	
Contribution identifier	8a5	
Measurement equation parameter(s) subject to effect	-	
Contribution subject to effect (final product or sub-tree intermediate product)	Ventialtion speed	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	0	
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	No	

Validation	Ventilation speed validation experiments.	

5.21 Sensor orientation (8a10)

Due to the fact that the RS92 temperature sensor is a wire rather than a sphere, the direct solar flux onto the sensor depends on its orientation. The geometry factor g accounts for the reduction of the exposed area of the temperature sensor due to spinning of the radiosonde, which causes the orientation of the sensor wire to cycle between being parallel and perpendicular to the solar rays. Currently, a value of 0.5 is used for g, but this may change in the next version of the GRUAN processing.

Information / data	Type / value / equation	Notes / description
Name of effect	Sensor orientation	
Contribution identifier	8a10	
Measurement equation parameter(s) subject to effect	-	
Contribution subject to effect (final product or sub-tree intermediate product)	Radiation correction	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Static	
Uncertainty & units (1σ)	0	
Sensitivity coefficient	1	
Correlation(s) between affected parameters		
Element/step common for all sites/users?		
Traceable to …		
Validation		

5.22 Cloud configuration (8a11)

No separate contribution – the uncertainty is effectively included as part of the radiative model fit uncertainity (8a2).

Information / data	Type / value / equation	Notes / description

Name of effect	Cloud configuration	
Contribution identifier	8a11	
Measurement equation parameter(s) subject to effect	-	
Contribution subject to effect (final product or sub-tree intermediate product)	Actinic flux Radiative transfer model	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Static	
Uncertainty & units (1σ)	0	
Sensitivity coefficient	1	
Correlation(s) between affected parameters		
Element/step common for all sites/users?		
Traceable to …		
Validation		

5.23 **Albedo (8a12)** $u_{c,\,(Ia)}$ **&** $u_{u,\,Ia(\Delta T)}$

$$\Delta T \cdot u_{\mathrm{c}}(I_{\mathrm{a}})/I_{\mathrm{a}}$$

where ΔT is the solar radiation correction term and

$$u_c(I_a) = \frac{1}{2\cdot\sqrt{3}}\left|I_{\mathrm{a}}^{\text{clear sky}} - I_{\mathrm{a}}^{\text{cloudy}}\right|$$

Information / data	**Type / value / equation**	**Notes / description**
Name of effect	Albedo	
Contribution identifier	8a9	
Measurement equation parameter(s) subject to effect	Radiation correction temperature correction $\Delta T = a.\left(\frac{I_a}{p.v}\right)^b$ Where Albedo is used to determine I_a	
Contribution subject to effect (final product or sub-tree intermediate product)	Radiation correction	

Time correlation extent & form	Corrected point by point. correlates with time of day (SZA)	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Rectangular	
Uncertainty & units	Typical values are 0.2-0.5x ΔT in the trop. and 0.03-0.2x ΔT in the strat., so <0.05 K (2σ) throughout the ascent.	60-250 W/m^2 in the troposphere, 30-200 W/m^2 in the stratosphere dependant on SZA
Sensitivity coefficient	$\Delta T \sim {I_a}^b$	
Correlation(s) between affected parameters	SZA	
Element/step common for all sites/users?	Yes	
Traceable to …		
Validation		

5.24 Smoothing and spike removal (8b)

The smoothing and spike removal is covered by a series of three sub-processes: a low-pass filtering step (8b1), a positive outlier removal step (8b2) and a refiltering, interpolation and variability calculation (8b3). The uncertainty and correlation effects are covered in the sub-process sections.

Information / data	Type / value / equation	Notes / description
Name of effect	Smoothing and spike removal	
Contribution identifier	8b	
Measurement equation parameter(s) subject to effect	$T' = f(T),$	
Contribution subject to effect (final product or sub-tree intermediate product)	Temperature	
Time correlation extent & form	Filter width, 10s	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Quasi-rectangular	
Uncertainty & units (1σ)	±0.05K (2σ)	
Sensitivity coefficient	1	

Correlation(s) between affected parameters		
Element/step common for all sites/users?		
Traceable to …		
Validation		

5.25 Low pass filtering (8b1)

Low-pass filtering is applied over a 10 sec running average, reducing the vertical resolution to 50 m, although data is reported at 1 second intervals.

No uncertainty associated with this process is considered.

Information / data	**Type / value / equation**	**Notes / description**
Name of effect	Low pass filtering	
Contribution identifier	8b1	
Measurement equation parameter(s) subject to effect	$T' = f(T)$	
Contribution subject to effect (final product or sub-tree intermediate product)	Tempertaure	
Time correlation extent & form	Over filter width (10 sec)	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	0 K	
Sensitivity coefficient	1	
Correlation(s) between affected parameters	8b2	
Element/step common for all sites/users?	Yes	
Traceable to …	No	
Validation	No	

5.26 Positive outlier removal (8b2)

Spikes in the daytime temperature profile may result from air being heated by the radiosonde package, and possibly from passing through the warm wake of the balloon due to the pendulum motion of the payload[25,4].

Reduces the mean temperature, by removing positive outliers.

Information / data	Type / value / equation	Notes / description
Name of effect	Outlier correction	
Contribution identifier	8b2	
Measurement equation parameter(s) subject to effect	Temperature	
Contribution subject to effect (final product or sub-tree intermediate product)	Radiation correction (8)	
Time correlation extent & form	Correlated over smoothing kernel, 10sec	
Other (non-time) correlation extent & form	Correlated over smoothing kernel, 10sec	
Uncertainty PDF shape	Rectangular	
Uncertainty & units (1σ)	0.05K	
Sensitivity coefficient	1	
Correlation(s) between affected parameters		
Element/step common for all sites/users?	Yes	
Traceable to …	None	
Validation		

5.27 Refiltering, interpolation and variability calc. (8b3)

No uncertainty associated with the refiltering, interpolation & variability processing is considered.

Information / data	Type / value / equation	Notes / description
Name of effect	Refiltering & interpolation	
Contribution identifier	8b3	
Measurement equation parameter(s) subject to effect	$T' = f(T)$	
Contribution subject to effect (final product or sub-tree intermediate product)	Temperature	
Time correlation extent & form	Over filter width (10 sec)	

Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	0 K	
Sensitivity coefficient	1	
Correlation(s) between affected parameters	8b2	
Element/step common for all sites/users?	Yes	
Traceable to …	No	
Validation	No	

5.28 Sensor rotation (8c) $u_{u,\, rot(\Delta T)}$

Due to spinning of the radiosonde in flight, the solar irradiance on the sensor wire cycles between 0 and maximum. In case of rapid spinning – i.e. more than, say, 10 revolutions per minute – the temperature rise due to the orientation should average out and should not introduce a mean bias in the temperature profile. Not knowing the instantaneous rotational rate leads to an increased uncertainty around the mean radiation bias. However, if the radiosonde rotates slowly, the orientation of the temperature sensor with respect to the Sun no longer averages out.
The orientation uncertainty and the associated temperature uncertainty only apply to the direct solar irradiance is because the temperature error from the diffuse (omnidirectional) background remains largely the same regardless of sensor orientation. proportional to radiation correction calculated in 8a1.

Figure 10 shows the typical magnitude of the sensor rotation (orientation) uncertainty compared to the other major sources of uncertainty.

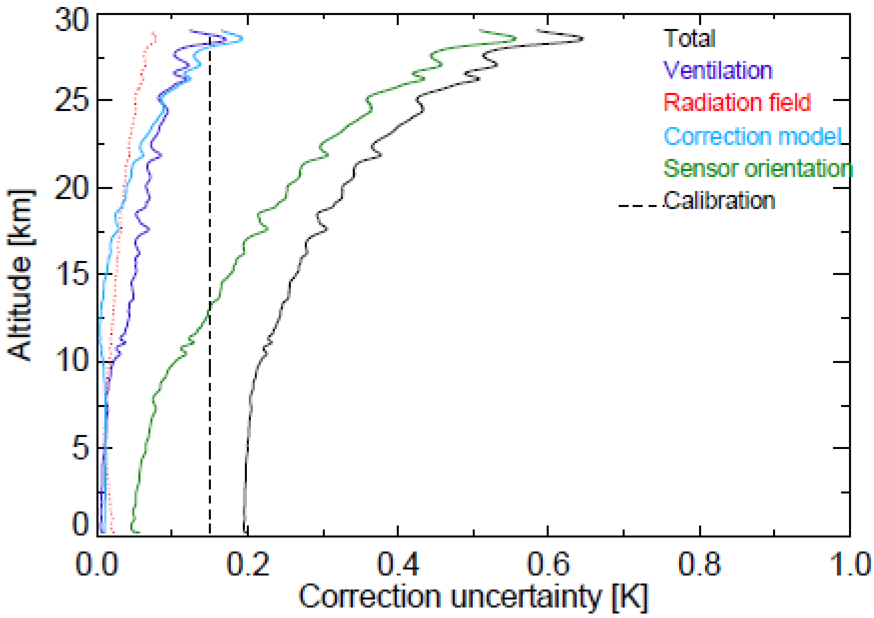


Figure 9. Contributions of the various uncertainty terms to the total uncertainty estimate of the GRUAN temperature correction for a sounding performed in Lindenberg on 17 September 2013 at 12:00 UTC; maximum solar zenith angle during the sounding: 36.5°. The radiation field represents the uncertainty due to the unknown albedo of the cloudy/cloud-free scene.

Figure 10. Dirksen et al[1] figure 9.

Information / data	Type / value / equation	Notes / description
Name of effect	Sonde rotation	
Contribution identifier	8c, $u_{u,\,rot(\Delta T)}$	
Measurement equation parameter(s) subject to effect	$u_{u,rot(\Delta T)} = 2.\frac{\Delta T}{\sqrt{3}}$	Where ΔT is the radiation correction.
Contribution subject to effect (final product or sub-tree intermediate product)	Temperature	
Time correlation extent & form	Corrected point by point.	
Other (non-time) correlation extent & form	Pressure & ventilation speed.	
Uncertainty PDF shape	Rectangular	As ΔT (8a2) is rectangular
Uncertainty & units (1σ)	±0.1 K (2σ) in trop. ±0.4 K (2σ) in strat. as a function of altitude & ventilation speed.	$u_{rot} = 2.\frac{\Delta T}{\sqrt{3}}$ Highest for low ventilation speed & high altitude.
Sensitivity coefficient	1	
Correlation(s) between affected parameters	Actinic flux inceratinty.	

Element/step common for all sites/users?	Yes	
Traceable to …		
Validation		

5.29 **Uncorrected uncertainty sources (9)**

The combination of the additional uncorrected uncertainty sources, sensor time lag (9a), evaporative cooling (9b) and payload configuration (9c), which are combined in the following way:

$$u_{uncor} = \sqrt{\left(u_{tlag}{}^{2} + u_{evap}{}^{2} + u_{payload}{}^{2}\right)}$$

Information / data	**Type / value / equation**	**Notes / description**
Name of effect	Uncorrected uncertainty sources	
Contribution identifier	9	
Measurement equation parameter(s) subject to effect	$T' = T$	Additional uncertainty alone
Contribution subject to effect (final product or sub-tree intermediate product)	Temperature	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Systematic	
Uncertainty & units (1σ)	0 K	
Sensitivity coefficient	1	
Correlation(s) between affected parameters	8a5 & 8b	
Element/step common for all sites/users?	Yes	
Traceable to …	No	
Validation	No	

5.30 **Sensor time lag (9a)**

The RS92 temperature sensors respond to changes in the ambient temperature, with typical time constants of 1.7 s at 3 hPa, 1.3 s at 10 hPa, and < 0:5 s below 100 hPa[3]. Sensors made prior to 2007 were slightly thinner and responded with time constants approximately 60% smaller (e.g. 1 s at 3 hPa). The response of the temperature sensor converges exponentially to changes in ambient temperature, and the time constant is the time needed to register 63% of a step change in temperature. These response times are fast enough to keep the temperature error due to sensor time-lag below 0.1 K. Therefore, no correction for time-lag of the temperature sensor is applied in the GRUAN product.

Information / data	Type / value / equation	Notes / description
Name of effect	Sensor time lag	
Contribution identifier	9a	
Measurement equation parameter(s) subject to effect	$T' = T$	Additional uncertainty alone
Contribution subject to effect (final product or sub-tree intermediate product)	Temperature	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Quasi-systematic	
Uncertainty & units (1σ)	0 K	
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	No	
Validation	No	

5.31 Evaporative cooling (9b)

When the radiosonde flies through a cloud, the temperature sensor will inevitably be coated with water or ice, which may introduce errors in the temperature measurements above the cloud due to evaporative cooling. In extreme cases this effect can cause the occurrence of apparent superadiabatic lapse rates (SLRs) in radiosonde profiles near cloud tops[25]. Inside the cloud, the condensate on the temperature sensor is close to equilibrium with the surrounding air, so it is unlikely to affect the temperature measurement. However, after exiting the cloud, condensate starts to evaporate, leading to evaporative cooling of the sensor until all water or ice has evaporated. The magnitude and vertical extent of the error due to evaporative cooling are difficult to quantify as they depend on the unknown amount and phase of the condensate deposited on the sensor, and on the temperature and humidity of the ambient air above the cloud. Vaisala uses a special hydrophobic coating for the temperature sensor and the sensor boom to make the RS92 less prone to evaporative cooling. Currently, the GRUAN processing does not correct for this effect. In the next version of the data processing, evaporative cooling will be detected by superadiabatic lapse rates that coincide with a rapid decrease of humidity away from (near) saturation. The uncertainty budget will be adjusted where these SLRs occur.

Information / data	Type / value / equation	Notes / description
Name of effect	Evaporative cooling	
Contribution identifier	9b	
Measurement equation parameter(s) subject to effect	$T' = T$	Additional uncertainty alone
Contribution subject to effect (final product or sub-tree intermediate product)	Temperature	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Quasi-systematic	
Uncertainty & units (1σ)	0 K	
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	No	
Validation	No	

5.32 Payload configuration (9c)

The payload configuration may introduce an additional error source. If a radiosonde is attached to a white Styrofoam ozone sonde box, this can act as a scattering surface and enhance the actinic flux on the temperature sensor in the same manner as clouds. A large object close to the radiosonde may also obstruct the proper ventilation of the temperature sensor. The GRUAN product does not employ a correction algorithm for the radiation and ventilation errors related to payload configuration. These errors are hard to quantify, and systematic experimental data to create such a correction is lacking. Therefore, in addition to the recommendations on the exposure of the temperature sensor given in chapter 12 of WMO (2008)[27], proper separation between neighbouring instruments within a payload should be considered, not only to ensure proper ventilation but also to minimize the additional radiation error.

Another effect of large payloads is the change of the rotation frequency of the rig, which changes the size and shape of the temperature spikes. The GRUAN spike algorithm removes all temperature spikes that exceed the threshold, provided the spike duration is short enough to be detected by the low-pass filter.

Information / data	Type / value / equation	Notes / description
Name of effect	Payload configuration	
Contribution identifier	9c	
Measurement equation parameter(s) subject to effect	$T' = T$	Additional uncertainty alone
Contribution subject to effect (final product or sub-tree intermediate product)	Temperature	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Systematic (over ascent)	
Uncertainty & units (1σ)	0 K	
Sensitivity coefficient	1	
Correlation(s) between affected parameters	Ventilation speed 8a5 & spike removal 8b	
Element/step common for all sites/users?	Yes	
Traceable to …	No	
Validation	No	

6 Uncertainty Summary

Element identifier	Contribution name	Uncertainty contribution form	Typical value	Traceability level (L/M/H)	random, structured random, quasi-systematic or systematic?	Correlated to? (Use element identifier)
1	**Capacitive sensor**	**Accuracy** **statistical uncertainty** $\sigma(T)/\sqrt{N'}$	**±0.5 K (2σ)** **±0.1 K (1σ) in the trop. 0.2-0.5 K (1σ) in strat.**	**H** **H**	**Systematic (over ascent)** **random**	**none**
2	**Vaisala CAL4 calibration repeatability**	**constant**	**±0.15K (2σ)**	**H**	**random**	**none**
2a	Reference T sensor accuracy	constant	<±0.1 K (2σ)	H	systematic	none
3	**Transport & storage**	**constant**	**0 K**	**L**	**systematic**	**none**
4	**GC25 ground check pass/fail**	**Rectangular**	**0 K**	**M**	**systematic**	**2a**
5	**GC25 one point re-calibration**	**constant**	**±0.16 K (1σ)**	**H**	**systematic**	**2 & 5a**
5a	GC25 PT100 T sensor accuracy	constant	±0.15 K (1σ)	H	systematic	none
6	**Measurement time frame**	**N/A**	**0 K**	**H**	**random**	**none**
7	**Data transmitted to station**	**N/A**	**0 K**	**H**	**random**	**none**
8	**Post-measurement corrections**	**Primarily α ΔT (solar radiation correction)**	**±0.22 K (2σ) in trop. ±0.5 K (2σ) in strat.**	**M**	**quasi-systematic**	**none**
8a	Radiation correction	constant	<0.36 K (2σ)	M	systematic	none
8a1	Solar radiation temperature model	constant	<0.2 K (2σ)	M	systematic	none
8a2	Vaisala radiation correction	constant	0 K	M	quasi-systematic	8a1
8a3	Pressure	$\Delta T(I_a, p, v) = a \cdot x^b$ with $x = \frac{I_a}{p \cdot v}$	<0.001 K (1σ) in the trop., rising to ±0.03 K (1σ) in the strat.	M	random	Pressure product & 8a10
8a4	Solar Zenith Angle	constant	0 K	M	Systematic (over ascent)	
8a5	Launch site location	constant	0 K	H	Systematic	

8a6	Time of launch	constant	0 K	H	Systematic (over ascent)	
8a7	Actrinic flux model	constant	0 K	M	quasi-systematic	none
8a8	Ventilation speed	constant	±0.01 K (2σ) in the trop. up to ±0.3 K (2σ) in the strat.	M	quasi-systematic	Altitude product
8a9	Altitude	constant	0 K	M	quasi-systematic	Altitude product
8a10	Sensor orientation	constant	0 K	M	systematic	8a1
8a11	Cloud configuration	constant	0 K	L	Systematic	
8a12	Albedo	$\Delta T \cdot u_{\mathrm{c}}(I_{\mathrm{a}})/I_{\mathrm{a}}$ where ΔT is the solar radiation correction term from 8a1 and $\mathrm{U_c(I_a)} = \frac{1}{2\cdot\sqrt{3}}\lvert I_{\mathrm{a}}^{\text{clear sky}} - I_{\mathrm{a}}^{\text{cloudy}}\rvert$	<0.05K (2σ)	M	Systematic (over ascent)	none
8b	Smoothing & spike removal	constant	±0.05K (2σ)	M	quasi-systematic	2
8b1	Low pass filtering	constant	0 K	M	quasi-systematic	2
8b2	Positive outlier removal	constant	±0.05K (2σ)	M	quasi-systematic	2
8b3	Refiltering, interpolation & variability	constant	0 K	M	quasi-systematic	2
8c	Rotating sonde	$2 \cdot \Delta T/\sqrt{3}$ where ΔT is the solar radiation corr.	±0.1 K (2σ) in trop. ±0.4 K (2σ) in strat.	M	quasi-systematic	
9	**Additional uncorrected sources**	**constant**	**<0.2K (2σ)**	**M**	**Systematic (over ascent)**	**8a5 & 8b**
9a	Sensor time lag	constant	< 0.03K (2σ)	M	quasi-systematic	none
9b	Evaporative cooling	constant	<0.2K (2σ)	M	Systematic (over ascent)	none
9c	Payload configuration	constant	0 K	L	Systematic	8a5 & 8b

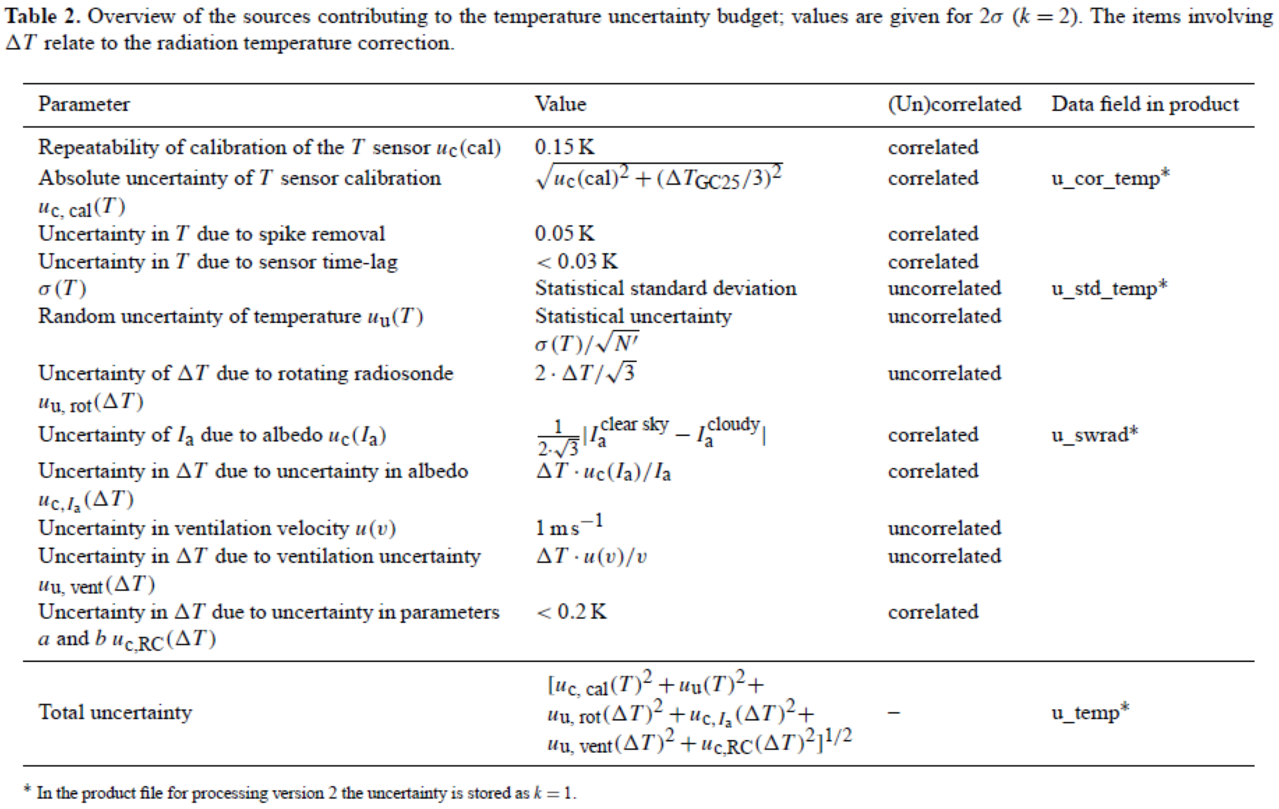


Table 2. Overview of the sources contributing to the temperature uncertainty budget; values are given for 2σ ($k = 2$). The items involving ΔT relate to the radiation temperature correction.

Parameter	Value	(Un)correlated	Data field in product
Repeatability of calibration of the T sensor $u_\mathrm{c}(\mathrm{cal})$	0.15 K	correlated	
Absolute uncertainty of T sensor calibration $u_\mathrm{c,\,cal}(T)$	$\sqrt{u_\mathrm{c}(\mathrm{cal})^2 + (\Delta T_\mathrm{GC25}/3)^2}$	correlated	u_cor_temp*
Uncertainty in T due to spike removal	0.05 K	correlated	
Uncertainty in T due to sensor time-lag	< 0.03 K	correlated	
$\sigma(T)$	Statistical standard deviation	uncorrelated	u_std_temp*
Random uncertainty of temperature $u_\mathrm{u}(T)$	Statistical uncertainty $\sigma(T)/\sqrt{N'}$	uncorrelated	
Uncertainty of ΔT due to rotating radiosonde $u_\mathrm{u,\,rot}(\Delta T)$	$2 \cdot \Delta T/\sqrt{3}$	uncorrelated	
Uncertainty of I_a due to albedo $u_\mathrm{c}(I_\mathrm{a})$	$\frac{1}{2\cdot\sqrt{3}}\lvert I_\mathrm{a}^\mathrm{clear\ sky} - I_\mathrm{a}^\mathrm{cloudy}\rvert$	correlated	u_swrad*
Uncertainty in ΔT due to uncertainty in albedo $u_{\mathrm{c},I_\mathrm{a}}(\Delta T)$	$\Delta T \cdot u_\mathrm{c}(I_\mathrm{a})/I_\mathrm{a}$	correlated	
Uncertainty in ventilation velocity $u(v)$	$1\,\mathrm{m\,s^{-1}}$	uncorrelated	
Uncertainty in ΔT due to ventilation uncertainty $u_\mathrm{u,\,vent}(\Delta T)$	$\Delta T \cdot u(v)/v$	uncorrelated	
Uncertainty in ΔT due to uncertainty in parameters a and b $u_\mathrm{c,RC}(\Delta T)$	< 0.2 K	correlated	
Total uncertainty	$[u_\mathrm{c,\,cal}(T)^2 + u_\mathrm{u}(T)^2 +$ $u_\mathrm{u,\,rot}(\Delta T)^2 + u_{\mathrm{c},I_\mathrm{a}}(\Delta T)^2 +$ $u_\mathrm{u,\,vent}(\Delta T)^2 + u_\mathrm{c,RC}(\Delta T)^2]^{1/2}$	–	u_temp*

* In the product file for processing version 2 the uncertainty is stored as $k = 1$.

Figure 11. Uncertainty summary table from Dirksen et al[1].

The contribution of the major uncertainty sources is summarised in Figure 11. The altitude dependence of these is shown in Figure 10.

The combination of uncertainties is given by

$$[\boldsymbol{u}_{c,cal}(\boldsymbol{T})^2 + \boldsymbol{u}_u(\boldsymbol{T})^2 + \boldsymbol{u}_{u,rot}(\boldsymbol{T})^2 + \boldsymbol{u}_{c,I_a}(\boldsymbol{T})^2 + \boldsymbol{u}_{u,vent}(\boldsymbol{T})^2 + \boldsymbol{u}_{c,RC}(\boldsymbol{T})^2]^{1/2}$$

Where

$U_{c,\ cal(T)} =$ $\sqrt{u_\mathrm{c}(\mathrm{cal})^2 + (\Delta T_\mathrm{GC25}/3)^2}$

giving typical daytime uncertainties of ±0.62 K (2σ) in the troposphere and ±0.92 K (2σ) in the stratosphere.

7 Traceability uncertainty analysis

Traceability level definition is given in Table 2.

Table 2. Traceability level definition table

Traceability Level	Descriptor	Multiplier
High	SI traceable or globally recognised community standard	1
Medium	Developmental community standard or peer-reviewed uncertainty assessment	3
Low	Approximate estimation	10

Analysis of the summary table would suggest the following contributions, shown in Table 3, should be considered further to improve the overall uncertainty of the GRUAN temperature product. The entires are given in an estimated priority order.

Table 3. Traceability level definition further action table.

Element identifier	Contribution name	Uncertainty contribution form	Typical value	Traceability level (L/M/H)	random, structured random, quasi-systematic or systematic?	Correlated to? (Use element identifier)
8a2	Vaisala radiation correction	constant	0 K	M	quasi-systematic	8a1
8c	Rotating sonde	$2 \cdot \Delta T / \sqrt{3}$ where ΔT is the solar radiation corr.	±0.1 K (2σ) in trop. ±0.4 K (2σ) in strat.	M	quasi-systematic	
8a8	Ventilation speed	constant	±0.01 K (2σ) in the trop. up to ±0.3 K (2σ) in the strat.	M	quasi-systematic	Altitude product
8a9	Altitude	constant	0 K	M	quasi-systematic	Altitude product
3	Transport & storage	constant	0 K	L	systematic	none
4	GC25 ground check pass/fail	Rectangular	0 K	M	systematic	2a
8a4	Solar Zenith Angle	constant	0 K	M	Systematic (over ascent)	
8a5	Launch site location	constant	0 K	H	Systematic	
8a6	Time of launch	constant	0 K	H	Systematic (over ascent)	
8a7	Actrinic flux model	constant	0 K	M	quasi-systematic	none

8a10	Sensor orientation	constant	0 K	M	systematic	8a1
8a11	Cloud configuration	constant	0 K	L	Systematic	
8b1	Low pass filtering	constant	0 K	M	quasi-systematic	2
8b3	Refiltering, interpolation & variability	constant	0 K	M	quasi-systematic	2

7.1 Recommendations

An assessment of the uncertainty of the Vaisala solar heating correction term (8a2) should be evaluated.

Rotating sonde (8c) and Ventiation speed (8a8) are major contributors to the stratospheric tempertaure uncertainty which, with further investigation, could potentially be improved.

There are 11 contributions that do not have an assigned uncertainty. Some analysis to determine the magnitude of these potential contributions1 would better constrain the uncertainty budget.

8 Conclusion

The GRUAN RS92 radiosonde temperature product has been assessed against the GAIA CLIM traceability and uncertainty criteria.

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Product Traceability and Uncertainty for the GRUAN RS92 radiosonde humidity product

Version 2.0

GAIA-CLIM
Gap Analysis for Integrated
Atmospheric ECV Climate Monitoring
Mar 2015 - Feb 2018

A Horizon 2020 project; Grant agreement: 640276

Date: 30 November 2017

Dissemination level: PU

Work Package 2; Complied by David Medland
Paul Green & Tom Gardiner (NPL)

Table of Contents

Version history

Version	Principal updates	Owner	Date
1.0	First issue	NPL	22.09.2017
2.0	Issued as annex C to D2.6	NPL	30.11.2017

1 Product overview

Product name: In-situ radiosonde RS92 relative humidity
Product technique: Capacitive humidity sensor
Product measurand: relative humidity
Product form/range: profile (ground to 30km, 1sec sampling)
Product dataset: GRUAN Reference level sonde dataset
Site/Sites/Network location:

SITE	LAT	LON	HEIGHT(m)	LOCATION	COUNTRY
BEL	39.05	-76.88	53	Beltsville	US
BOU	71.32	-156.61	8	Boulder	US
CAB	51.97	4.92	1	Cabauw	NL
LAU	-45.05	169.68	370	Lauder	NZ
LIN	52.21	14.12	98	Lindenberg	DE
NYA	78.92	11.92	5	Ny-Ålesund	NO
PAY	46.81	6.95	491	Payerne	CH
POT	40.60	15.72	720	Potenza	IT
SOD	67.37	26.63	179	Sodankylä	FI

Product time period: 20 May 2006 to present
Data provider: GRUAN
Instrument provider: Site operators, see www.gruan.org.
Product assessor: David Medland, NPL
Assessor contact email: david.medland@npl.co.uk

1.1 Guidance notes

For general guidance see the Guide to Uncertainty in Measurement & its Nomenclature, published as part of the GAIA-CLIM project.

This document is a measurement product technical document which should be stand-alone i.e. intelligible in isolation. Reference to external sources (preferably peer-reviewed) and documentation from previous studies is clearly expected and welcomed, but with sufficient explanatory content in the GAIA-CLIM document not to necessitate the reading of all these reference documents to gain a clear understanding of the GAIA-CLIM product and associated uncertainties entered into the Virtual Observatory (VO).

In developing this guidance, we have created a convention for the traceability identifier numbering as shown in Figure 1. The 'main chain' from raw measurand to final product forms the axis of the diagram, with top level identifiers (i.e. 1, 2, 3 etc.). Side branch processes add sub-levels components to the top level identifier (for example, by adding alternate letters & numbers, or 1.3.2 style nomenclature).

The key purpose of this sub-level system is that all the uncertainties from a sub-level are summed in the next level up.

For instance, using Figure 1, contributors 2a1, 2a2 and 2a3 are all assessed as separate components to the overall traceability chain (have a contribution table). The contribution table for (and uncertainty associated with) 2a, should combine all the sub-level uncertainties (and any additional uncertainty intrinsic to step 2a). In turn, the contribution table for contributor 2, should include all uncertainties in its sub-levels.

Therefore, only the top level identifiers (1, 2, 3, etc.) shown in bold in the summary table need be combined to produce the overall product uncertainty. The branches can therefore be considered in isolation, for the more complex traceability chains, with the top level contribution table transferred to the main chain. For instance, see Figure 2 & Figure 3 as an example of how the chain can be divided into a number of diagrams for clearer representation.

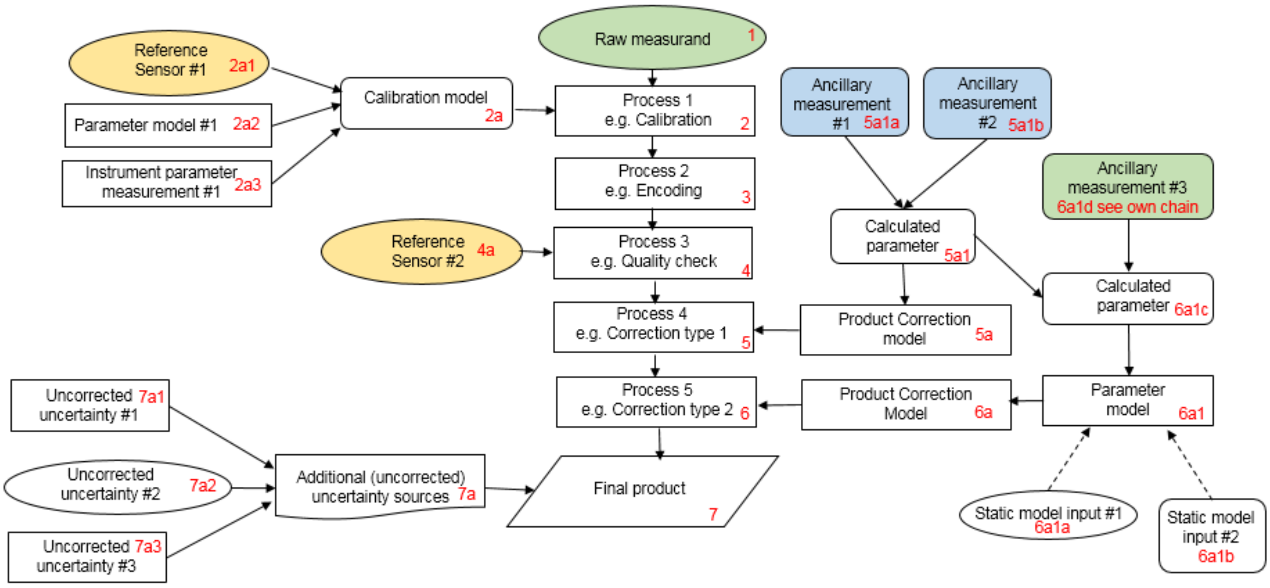


Figure 1. Example traceability chain. Green represents a key measurand or ancillary measurand recorded at the same time with the product raw measurand. Yellow represents a source of traceability. Blue represents a static ancillary measurement

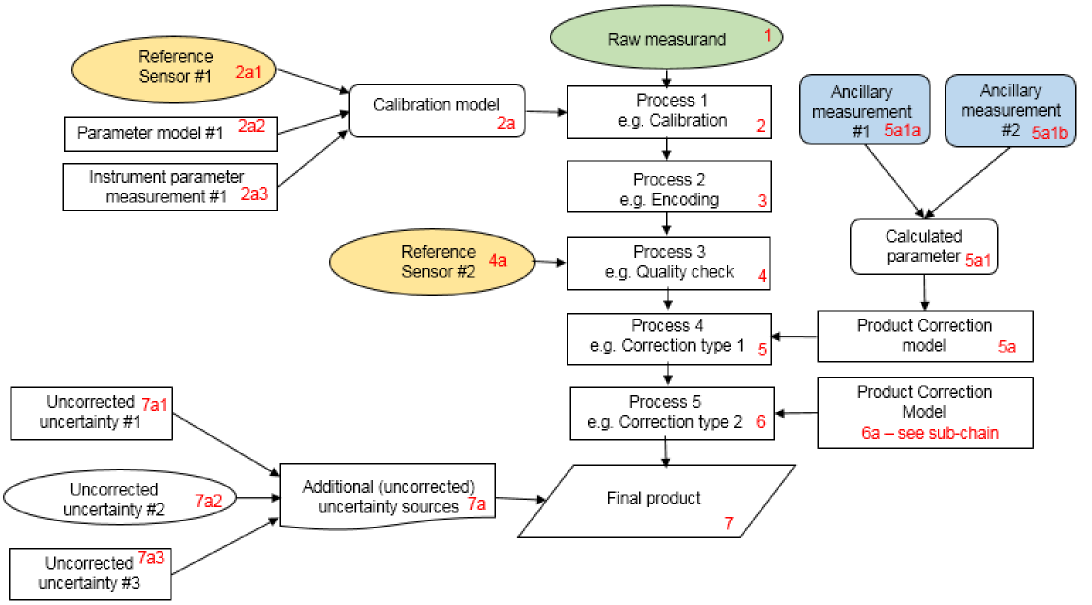


Figure 2. Example chain as sub-divided chain. Green represents a key measurand or ancillary measurand recorded at the same time with the product raw measurand. Yellow represents a source of traceability. Blue represents a static ancillary measurement

When deciding where to create an additional sub-level, the most appropriate points to combine the uncertainties of sub-contributions should be considered, with additional sub-levels used to illustrate where their contributions are currently combined in the described process.

A short note on colour coding. Colour coding can/should be used to aid understanding of the key contributors, but we are not suggesting a rigid framework at this time. In Figure 1, green represents a key measurand or ancillary or complementary measurand recorded at the same time with the raw measurand; yellow represents a primary source of traceability & blue represents a static ancillary measurement (site location, for instance). Any colour coding convention you use, should be clearly described.

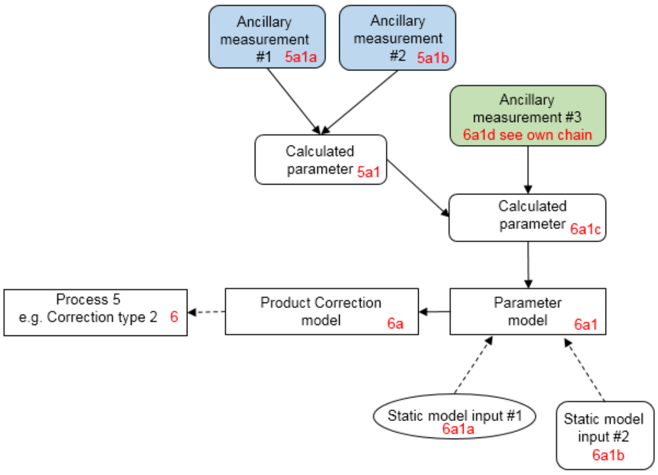


Figure 3. Example chain contribution 6a sub-chain. Green represents a key measurand or ancillary measurand recorded at the same time with the product raw measurand. Blue represents a static ancillary measurement

The contribution table to be filled for each traceability contributor has the form seen in Table 1.

Table 1. The contributor table.

Information / data	Type / value / equation	Notes / description
Name of effect		
Contribution identifier		
Measurement equation parameter(s) subject to effect		
Contribution subject to effect (final product or sub-tree intermediate product)		
Time correlation extent & form		
Other (non-time) correlation extent & form		
Uncertainty PDF shape		
Uncertainty & units		
Sensitivity coefficient		
Correlation(s) between affected parameters		
Element/step common for all sites/users?		
Traceable to …		
Validation		

Name of effect – The name of the contribution. Should be clear, unique and match the description in the traceability diagram.

Contribution identifier - Unique identifier to allow reference in the traceability chains.

Measurement equation parameter(s) subject to effect – The part of the measurement equation influenced by this contribution. Ideally, the equation into which the element contributes.

Contribution subject to effect – The top level measurement contribution affected by this contribution. This can be the main product (if on the main chain), or potentially the root of a side branch contribution. It will depend on how the chain has been sub-divided.

Time correlation extent & form – The form & extent of any correlation this contribution has in time.

Other (non-time) correlation extent & form – The form & extent of any correlation this contribution has in a non-time domain. For example, spatial or spectral.

Uncertainty PDF shape – The probability distribution shape of the contribution, Gaussian/Normal Rectangular, U-shaped, log-normal or other. If the form is not known, a written description is sufficient.

Uncertainty & units – The uncertainty value, including units and confidence interval. This can be a simple equation, but should contain typical values.

Sensitivity coefficient – Coefficient multiplied by the uncertainty when applied to the measurement equation.

Correlation(s) between affected parameters – Any correlation between the parameters affected by this specific contribution. If this element links to the main chain by multiple paths within the traceability chain, it should be described here. For instance, SZA or surface pressure may be used separately in a number of models & correction terms that are applied to the product at different points in the processing. See Figure 1, contribution 5a1, for an example.

Element/step common for all sites/users – Is there any site-to-site/user-to-user variation in the application of this contribution?

Traceable to – Describe any traceability back towards a primary/community reference.

Validation – Any validation activities that have been performed for this element?

The summary table, explanatory notes and referenced material in the traceability chain should occupy <= 1 page for each element entry. Once the summary tables have been completed for the full end-to-end process, the uncertainties can be combined, allowing assessment of the combined uncertainty, relative importance of the contributors and correlation scales both temporally and spatially. The unified form of this technical document should then allow easy comparison of techniques and methods.

2 Introduction

This document contains the product traceability and uncertainty information for the Global Climate Observing System (GCOS) Reference Upper-Air Network (GRUAN) Vaisala RS92 radiosonde relative humidity product.

The RS92 radiosonde measure relative humidity using two Humicaps which contain a hydro active polymer thin-film dielectric between two electrodes on a glass substrate. There is no protective cap on the humidity sensor but the two Humicaps are alternately heated to prevent icing. This heating is switched off below -60 ^{o}C or above 100 hPa, whichever is reached first, to prevent overheating. The Humicaps are initially calibrated at Vaisala's CAL4 facility and before launch there is a ground check with a GC25 unit and ideally a second ground check using a Standard Humidity Chamber (SHC). The raw relative humidity data is corrected for a temperature-related dry bias, radiative heating of the sensor and time lag experienced by the sensor at low temperatures. Vaisala and GRUAN processing both use the Hyland and Wexler 1983 formulation of saturation vapour pressure over water.

The GRUAN data processing was developed to meet the requirements of reference measurements including the collection of metadata, documentation of applied algorithms and estimates of uncertainty. The process by which the GRUAN processing collects raw relative humidity data as well as the calibrations and corrections applied are described in the paper Dirksen et al. 2014, which has been used in the creation of this document. The estimates for uncertainty provided here are those given in Dirksen et al. 2014[1] except in the case of elements where no uncertainty estimate is given where they have been calculated using the methods they describe. Dirksen et al. gives an estimate for total uncertainty in relative humidity of ±6 % RH.

3 Product Traceability Chain

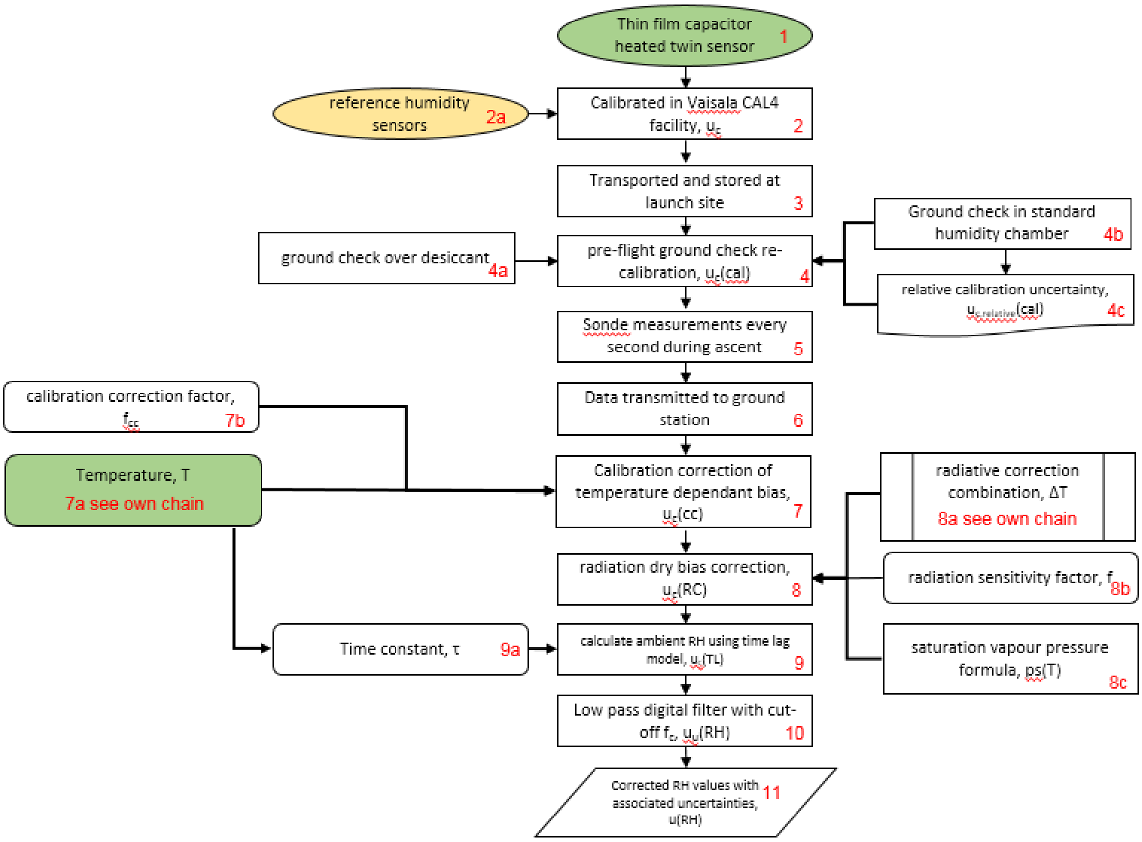


Figure 4 the traceability chain of the GRUAN relative humidity product excluding the radiative correction sub chain.

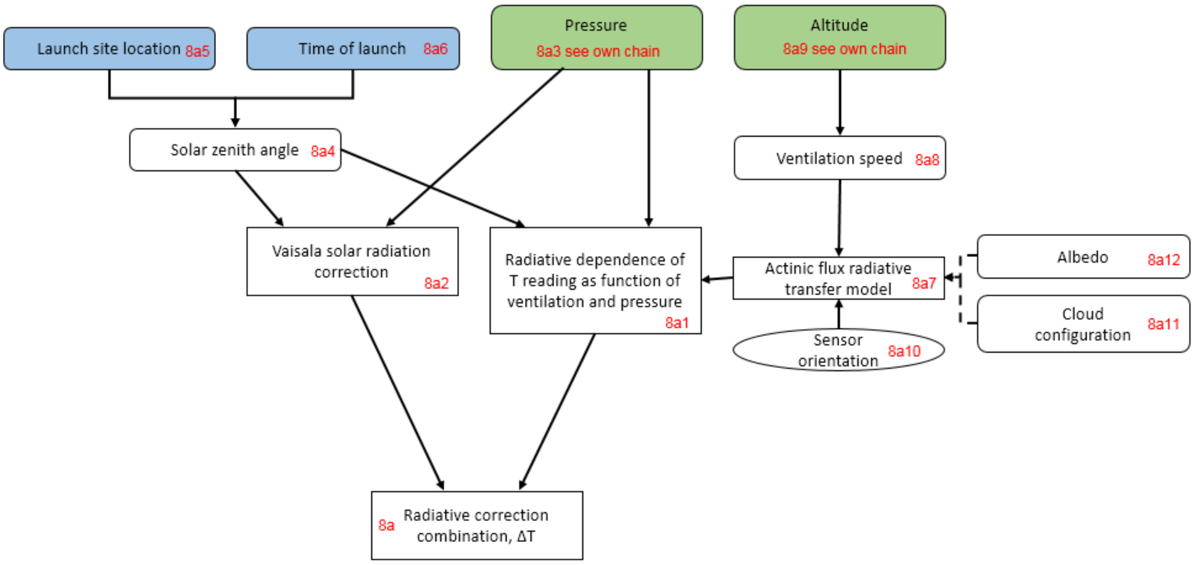


Figure 5 the radiative correction sub chain of the traceability chain for the GRUAN relative humidity product.

4 Element Contributions

4.1 Thin film capacitor heated twin sensor (1)

The Vaisala RS92 radiosonde carries two thin film polymer capacitive moisture sensors and the measurements from these sensors are merged. These have a thin polymer layer between two porous electrodes. Water molecules are captured at binding sites in the polymer, altering the capacitance of the sensor. The number of occupied binding sites is proportional to the ambient air water vapour density. The sensors have a measurement range of 0 to 100 % RH and a resolution of 1 % RH.

The uncertainty shown here is the reproducibility in soundings determined by Vaisala using the standard deviation between twin soundings as determined by Vaisala[2], although it is not used in the GRUAN product uncertainty, but GRUAN calculate the equivalent elsewhere in 10.

Information / data	Type / value / equation	Notes / description
Name of effect	Thin film capacitor heated twin sensor reproducibility	Multiple sounding std dev.
Contribution identifier	1	
Measurement equation parameter(s) subject to effect	Relative Humidity. RH' = RH	
Contribution subject to effect (final product or sub-tree intermediate product)	Relative Humidity.	
Time correlation extent & form	point-to-point	
Other (non-time) correlation extent & form	None.	
Uncertainty PDF shape	Normal.	
Uncertainty & units (2σ)	2 % RH	Reproducibility in sounding.
Sensitivity coefficient	1	Not used in the GRUAN uncertainty calculation. An equivalent calculated in step 10 is used instead.
Correlation(s) between affected parameters	None.	
Element/step common for all sites/users?	Yes	
Traceable to …	Vaisala	
Validation		

4.2 Calibrated in Vaisala CAL4 facility (2), u_c

Vaisala's CAL4 calibration facility has four chambers dedicated to humidity calibration operating at relative humidities between 0 % RH and over 90 % RH and a fifth chamber used to check humidity readings at low temperatures. Dew point meters which are calibrated every 12 months are used as humidity measurement references (see 2a). The relative humidity of the chambers are calculated using the measured dew point temperature and chamber temperature. The temperature references are calibrated every 6 months[3].

The calibration uncertainty is determined by Vaisala using the measurement uncertainties and the process uncertainties.

Information / data	Type / value / equation	Notes / description
Name of effect	Calibrated in Vaisala CAL4 facility	
Contribution identifier	2, u_c	
Measurement equation parameter(s) subject to effect	Relative Humidity RH' = aRH + b	Assumed measurement equation
Contribution subject to effect (final product or sub-tree intermediate product)	Relative Humidity	
Time correlation extent & form	Long term	Reference hygrometers are calibrated every 12 months.
Other (non-time) correlation extent & form	Over sounding	
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	2 % RH	Repeatability in calibration
Sensitivity coefficient	1	
Correlation(s) between affected parameters	none	
Element/step common for all sites/users?	Yes	
Traceable to …	Reference humidity sensors.	2a
Validation		

4.3 Reference Humidity Sensors (2a)

High precision dewpoint hygrometers are used as reference sensors for humidity. These are calibrated every 12 months in the Finnish National Measurements Standards Laboratory for Humidity (MIKES)[3].

Figure 6 shows the year-on-year variation in calibration bias for each batch of Vaisala sondes.

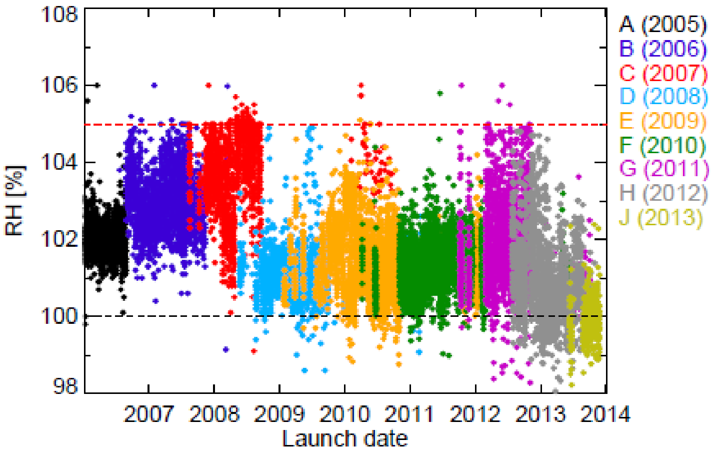


Figure 12. Time series of reading of the RS92 humidity sensor when inserted in the SHC (100 % relative humidity) prior to launch, as part of the additional manufacturer-independent ground check. The colours depict the radiosonde's production year. The black dashed line represents the 100 % level, whereas the red dashed line indicates 105 %, the rejection criterion for humidity readings in the SHC.

Figure 6. Dirksen 2014, figure 12.

Information / data	Type / value / equation	Notes / description
Name of effect	Reference humidity sensors.	
Contribution identifier	2a	
Measurement equation parameter(s) subject to effect	Relative Humidity RH' = RH	
Contribution subject to effect (final product or sub-tree intermediate product)	Calibration in CAL4 facility.	
Time correlation extent & form	Long term	Calibrated every 12 months, temperature references calibrated every 6 months
Other (non-time) correlation extent & form	Over sounding	
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	0.8 % RH @ 0 % RH to 90 % RH calibration. 1.2 % RH, 30 % RH at -33 °C check.	From Vaisala 2002.
Sensitivity coefficient	unknown	Included in given Vaisala calibration uncertainty.
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes.	
Traceable to …	MIKES	http://www.mikes.fi/en/services-

		for-industry/calibration-services
Validation		

4.4 Transported and stored at Launch Site (3)

Impurities can build up on the RS92 sensor boom during storage but these should be removed by heating the sensor boom before launch. Therefore in the GRUAN data processing it is assumed that transportation and storage do not attribute to the uncertainty of the measurements [1].

Information / data	Type / value / equation	Notes / description
Name of effect	Transported and stored at launch site.	
Contribution identifier	3	
Measurement equation parameter(s) subject to effect	Relative Humidity	
Contribution subject to effect (final product or sub-tree intermediate product)	Relative Humidity	
Time correlation extent & form	none	Proportional to length of storage
Other (non-time) correlation extent & form	none	
Uncertainty PDF shape	none	
Uncertainty & units (1σ)	0	
Sensitivity coefficient	0	
Correlation(s) between affected parameters	none	
Element/step common for all sites/users?	Yes.	
Traceable to …	n/a	
Validation		

4.5 Pre-flight Ground Check Recalibration (4), u_c(cal)

The GRUAN ground check includes a check over desiccant using the Vaisala GC25 unit and an advised check using a Standard Humidity Chamber (SHC). The uncertainty in the ground check calibration is calculated from these ground checks and from Vaisalas initial calibration. If no ground check is performed the uncertainty defaults to 4 % RH.

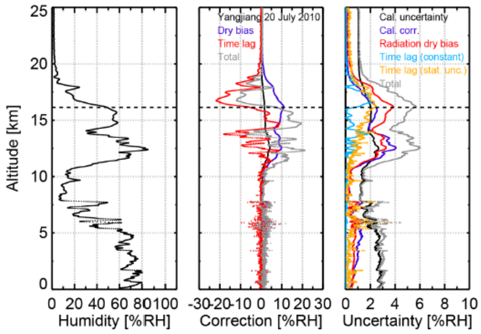


Figure 16. Corrections and their estimated uncertainties to the relative humidity. Left panel: humidity profile. Middle panel: profiles of the corrections for the temperature-dependent calibration correction (black), radiation dry bias (blue), and time-lag (red). The grey trace represents the total correction. Right panel: estimates of the total uncertainty (grey) and the various contributions due to the correction for calibration uncertainty (black), the correction for the temperature-dependent calibration correction (blue), radiation dry bias (red), time-lag constant $u(\tau)$ (light blue), and the statistical uncertainty of the time-lag correction (orange). The horizontal dashed line at 16.1 km represents the tropopause.

Figure 7 Dirksen 2014, figure 16

Information / data	Type / value / equation	Notes / description
Name of effect	Pre-flight Ground check recalibration	
Contribution identifier	4, $u_c(Cal)$	
Measurement equation parameter(s) subject to effect	Relative Humidity	
Contribution subject to effect (final product or sub-tree intermediate product)	Relative Humidity	
Time correlation extent & form	Long term	Between replacement of the desiccant used in the GC25 unit.
Other (non-time) correlation extent & form	Over sounding	
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	$u_c(Cal) = \sqrt{u_c^2 + u_{c,GC25}^2 + u_{c,absolute\ SHC}^2 + u_{c,relative}^2}(Cal)RH$	2-3 % RH, from Dirksen et al. figure 16, see figure 4.
Sensitivity coefficient	1	

Correlation(s) between affected parameters		
Element/step common for all sites/users?	yes	
Traceable to …	Vaisala calibration, GC25, SHC	
Validation		

4.6 Ground Check over Desiccant (4a), $u_{c,GC25}$

The readings of the radiosonde over a desiccant in near 0 % RH are used to determine possible drifts in the calibration of the sensors. The sensor readings are usually around 0.1 % RH after the desiccant is replaced but drift over time up to 1 % RH, indicating that they can detect the degradation of the desiccant. Because of this the ground check readings are not used to recalibrate the humidity sensors as in the standard Vaisala data processing, but are used in quality checks and the uncertainty estimate.

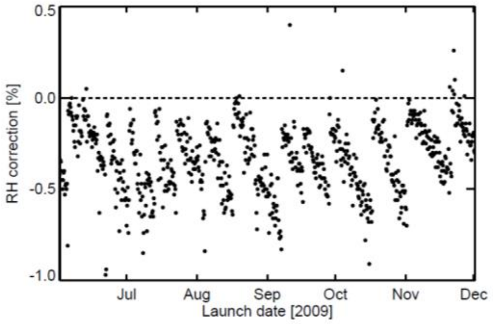


Figure 11. RH-sensor recalibration during ground check in the GC25 for RS92 radiosondes launched at Lindenberg in the second half of 2009. The desiccant is replaced bi-weekly, or when the recalibration exceeds 1 % RH.

Figure 8 Dirksen 2014, figure 11

Information / data	Type / value / equation	Notes / description
Name of effect	Ground check over desiccant	
Contribution identifier	4a, $u_{c,GC25}$	
Measurement equation parameter(s) subject to effect	Corrected RH values with associated uncertainty	
Contribution subject to effect (final product or sub-tree intermediate product)	Pre-flight ground check recalibration	
Time correlation extent & form	Long term	Over length of time between replacement of the desiccant.
Other (non-time) correlation extent & form	Over sounding	
Uncertainty PDF shape	rectangular	

Uncertainty & units (2σ)	$u_{c,GC25} = \sqrt{(\frac{\Delta U_1}{3})^2 + (\frac{\Delta U_2}{3})^2 + (U_1 - U_2)^2_{GC25}}$	<1 % RH. ΔU is usually less than 0.5 % RH. (Dirksen et al figure 11, see figure 5).
Sensitivity coefficient	1	
Correlation(s) between affected parameters		
Element/step common for all sites/users?	Yes	
Traceable to …		
Validation		

4.7 Ground check in Standard Humidity Chamber (4b), $u_{c,\mathrm{absolute\ SHC}}$

The SHC contains saturated (100 % RH) air above distilled water. Supersaturation is not expected because of condensation nuclei present in the ambient air. The uncertainty determined from the SHC check has an absolute and relative part. The absolute part is calculated from the difference between the two humidity sensor readings while in the SHC. Using a SHC during ground check is advised but not possible at every GRUAN site. In cases where the SHC check is not possible, 2.5 % RH is added to the calibration uncertainty.

Information / data	Type / value / equation	Notes / description
Name of effect	Ground check in standard humidity chamber	
Contribution identifier	4b, $u_{c,\mathrm{absolute\ SHC}}$	
Measurement equation parameter(s) subject to effect	Relative Humidity	
Contribution subject to effect (final product or sub-tree intermediate product)	Pre-flight ground check re-calibration	
Time correlation extent & form	none	
Other (non-time) correlation extent & form	Over sounding	
Uncertainty PDF shape	Triangular	
Uncertainty & units (2σ)	$u_{c,absolute\ SHC} = \sqrt{(U_1 - U_2)^2_{SHC}}$	U can be between 99 % RH and 105 % RH (Dirksen et al. figure 12, see figure 2).
Sensitivity coefficient	1	
Correlation(s) between affected parameters	Relative calibration uncertainty	
Element/step common for all sites/users?	no	A pre-flight check using a SHC is recommended but not possible at every site.

Traceable to …		
Validation		

4.8 Relative Calibration uncertainty (4_c) $u_{c,relative}$(cal)

The relative calibration uncertainty is using the difference between the readings of the two humidity sensors inside the SHC and the expected reading of 100 % RH.

Information / data	Type / value / equation	Notes / description
Name of effect	Relative calibration uncertainty	
Contribution identifier	4c, $u_{c,relative}$(cal)	
Measurement equation parameter(s) subject to effect	Relative Humidity	
Contribution subject to effect (final product or sub-tree intermediate product)	Pre-flight ground check re-calibration	
Time correlation extent & form	none	
Other (non-time) correlation extent & form	Throughout sounding	
Uncertainty PDF shape		
Uncertainty & units (2σ)	$u_{c,relative}(cal) = \sqrt{(U_1 - U_{SHC})^2 + (U_2 - U_{SHC})^2} / U_{SHC}$	Recently produced sondes usually have a U of <102 % RH (Dirksen et al. figure 12) and U_{SHC} = 100 %, giving an uncertainty of 0.028*RH.
Sensitivity coefficient	1	
Correlation(s) between affected parameters	Ground check in the Standard Humidity Chamber	
Element/step common for all sites/users?	No	
Traceable to …		
Validation		

4.9 Sonde measurements every second during ascent (5)

The uncertainty in these measurements is the statistical noise of the measurements, here represented by the standard deviation.

Information / data	Type / value / equation	Notes / description

Name of effect	Sonde measurements every second during ascent.	
Contribution identifier	5, σ(RH)	
Measurement equation parameter(s) subject to effect	Relative Humidity	
Contribution subject to effect (final product or sub-tree intermediate product)	Relative Humidity	
Time correlation extent & form	none	
Other (non-time) correlation extent & form	none	
Uncertainty PDF shape	normal	
Uncertainty & units (1σ)	0.5 – 1 % RH	Standard deviation of measurements.
Sensitivity coefficient	1	Not used in final combination
Correlation(s) between affected parameters	none	
Element/step common for all sites/users?	yes	
Traceable to …		
Validation		

4.10 Data Transmitted to Ground Station (6)

It is assumed there are no issues/uncertainties associated with data transmission from the radiosonde to the ground station.

Information / data	Type / value / equation	Notes / description
Name of effect	Data Transmitted to ground station.	
Contribution identifier	6	
Measurement equation parameter(s) subject to effect	Relative humidity	
Contribution subject to effect (final product or sub-tree intermediate product)	Relative humidity	
Time correlation extent & form	none	
Other (non-time) correlation extent & form	none	
Uncertainty PDF shape	none	
Uncertainty & units (1σ)	0 % RH	

Sensitivity coefficient	1	Not used in final combination
Correlation(s) between affected parameters	none	
Element/step common for all sites/users?	yes	
Traceable to …		
Validation		

4.11 Calibration Correction of Temperature Dependent Bias (7), $u_c(cc)$

The RS92 radiosonde has a temperature-dependant dry bias that cannot be attributed to radiative heating or time-lag and is attributed to inaccuracies in the Vaisala calibration of the humidity sensors[4]. This dry bias is predominantly between -40 and -60 °C and peaks at around -50 °C. The GRUAN processing corrects the dry bias by multiplying by a correction factor interpolated between reference points shown in table 1.

Table 2 Parameters for the temperature-dependent calibration correction of humidity values, from Dirksen et al. table 3.

Temperature (°C)	20	0	-15	-30	-50	-60	-70	-100
Correction Factor, f_{cc}	1.00	1.00	1.02	1.04	1.06	1.07	1.05	1.00
Uncertainty, $u(f_{cc})$	0.01	0.02	0.03	0.03	0.06	0.07	0.05	0.10

Information / data	Type / value / equation	Notes / description
Name of effect	Calibration of temperature dependent bias.	
Contribution identifier	7, $u_c(cc)$	
Measurement equation parameter(s) subject to effect	$RH^* = f_{cc}\,RH$	RH* are the corrected RH values.
Contribution subject to effect (final product or sub-tree intermediate product)	Relative humidity	
Time correlation extent & form	Long term	Between re-assessment of the correction factor
Other (non-time) correlation extent & form	Between reference temperatures.	
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	$u_c(cc) = \frac{u(f_{cc})}{f_{cc}} RH^*$	Usually about 2 % RH but can peak at 4 % RH.
Sensitivity coefficient	1	
Correlation(s) between affected parameters	Time lag correction	Both have a dependence on T.

Element/step common for all sites/users?	Yes	
Traceable to …		
Validation	Coincident frost-point hygrometer data	

4.12 Temperature (7a), T

The temperature is used to determine the correction factor that is applied to correct the temperature-dependent bias and to determine time constant used in the time-lag correction.

It is assumed that the uncertainty in temperature does not propagate into the uncertainty in relative humidity.

Information / data	Type / value / equation	Notes / description
Name of effect	Temperature	
Contribution identifier	7a, T	
Measurement equation parameter(s) subject to effect	f_{cc}, τ	
Contribution subject to effect (final product or sub-tree intermediate product)	Calibration correction of the temperature dependant bias, time lag correction	
Time correlation extent & form	Long term	
Other (non-time) correlation extent & form	Throughout sounding	
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	0.15 K (night time) 0.6 K (daytime)	0.02 % RH at night. 0.08 % RH at day.
Sensitivity coefficient	1	Not used in uncertainty assessment.
Correlation(s) between affected parameters	Time constant, τ Calibration correction factor, f_{cc}	
Element/step common for all sites/users?	yes	
Traceable to …	PTU of GRUAN temperature product	
Validation		

4.13 Calibration Correction Factor (7b)

The measured relative humidity is multiplied by a calibration correction factor to correct for the temperature-dependent dry bias.

Information / data	Type / value / equation	Notes / description
Name of effect	Calibration correction factor	
Contribution identifier	7b	
Measurement equation parameter(s) subject to effect	$RH^{*} = f_{cc}RH$	
Contribution subject to effect (final product or sub-tree intermediate product)	Calibration correction of temperature dependant bias	
Time correlation extent & form	Long term	
Other (non-time) correlation extent & form	Between reference temperatures	
Uncertainty PDF shape	rectangular	
Uncertainty & units (2σ)	0.01 to 0.10 unitless	See table 1
Sensitivity coefficient	RH^{*}/f_{cc}	
Correlation(s) between affected parameters		
Element/step common for all sites/users?	yes	
Traceable to …		
Validation		

4.14 Radiation dry bias correction (8), $u_c(RC)$

Solar radiation heats the humidity sensor and introduces a dry bias. Relative error can range from 9% at the surface to 50% at 15 km to correct this bias the measured profile is multiplied by a correction factor derived from the ratio of saturation pressure over water in the heated sensor and in ambient air.

$$RH_c = RH_m \frac{p_s(T + f\Delta T)}{p_s(T)}$$

The GRUAN processing uses the Hyland and Wexler 1983 formulation[5] for calculating saturation pressure over water. ΔT is the same as in the correction of the temperature product multiplied by a factor to represent the greater sensitivity of the humidity sensor to radiative warming. Because of this sections 3.15-3.27 are excerpted from the temperature PTU document, with some changes made to represent the humidity product.

Information / data	Type / value / equation	Notes / description
Name of effect	Radiation dry bias correction	
Contribution identifier	8	

Measurement equation parameter(s) subject to effect	$RH_c = RH_m \frac{p_s(T + f\Delta T)}{p_s(T)}$	
Contribution subject to effect (final product or sub-tree intermediate product)	Relative humidity	
Time correlation extent & form	Long term, between soundings.	
Other (non-time) correlation extent & form	Over profile	
Uncertainty PDF shape		
Uncertainty & units (2σ)	$u_c(RC) = \sqrt{u_c(RC_f)^2 + u_c(RC_t)^2}$	Can be over 5 % RH for mid-day launches but not present for night time soundings.
Sensitivity coefficient	1	
Correlation(s) between affected parameters	none	
Element/step common for all sites/users?	yes	
Traceable to …		
Validation		

4.15 Radiation correction combination (8a), ΔT

The radiative correction combination is the same as in the GRUAN temperature product. For daytime measurements it is the mean of the GRUAN and Vaisala radiation corrections but at nighttime only the Vaisala correction is used. Because the same temperature correction is used as in the temperature product, sections are the same as in the temperature product document.

Information / data	Type / value / equation	Notes / description
Name of effect	Radiation correction combination	
Contribution identifier	8a, ΔT	
Measurement equation parameter(s) subject to effect	$RH_c = RH_m \frac{p_s(T + f\Delta T)}{p_s(T)}$ Where $\Delta T = \frac{\Delta T_{GRUAN} + \Delta T_{Vaisala}}{2}$	
Contribution subject to effect (final product or sub-tree intermediate product)	Radiation dry bias correction	
Time correlation extent & form	Across soundings	
Other (non-time) correlation extent & form	Throughout profile	
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	$u_c(RC_T) =$	Low near the surface,

	$RH_m \frac{p_s(T+f(\Delta T+u(\Delta T)))-p_s(T+f(\Delta T-u(\Delta T)))}{2*p_s(T)}$	peaks at about 4 % RH near the tropopause for mid-day launches.
Sensitivity coefficient	1	
Correlation(s) between affected parameters	Radiation sensitivity factor	
Element/step common for all sites/users?	yes	
Traceable to …	Vaisala temperature correction	
Validation		

4.16 Radiative dependence of T reading as function of ventilation and pressure (8a1), $u_{c,RC(\Delta T)}$

During daytime the radiosonde sensor boom is heated by solar radiation, which introduces biases in temperature and humidity. The net heating of the temperature sensor depends on the amount of absorbed radiation and on the cooling by thermal emission and ventilation by air flowing around the sensor. Luers[6] used customized radiative transfer calculations and detailed information on the actual cloud configuration to accurately compute the radiation temperature error for selected soundings.

$$\Delta T(I_a, p, v) = a \cdot x^b \qquad \text{with } x = \frac{I_a}{p \cdot v},$$

a = 0:18 ± 0.03 and b = 0:55 ± 0:06, the uncertainty due to these parameters in a, b and the radiation correction is typically <0.2 K (2σ) daytime only. For nigh time the Vaisala correction of 0.04 K at 5 hPa is used.

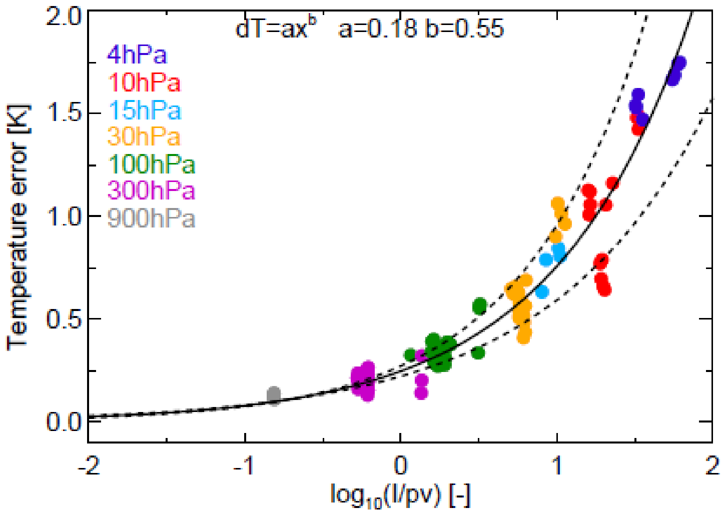


Figure 9. Dirksen et al[1] figure 4

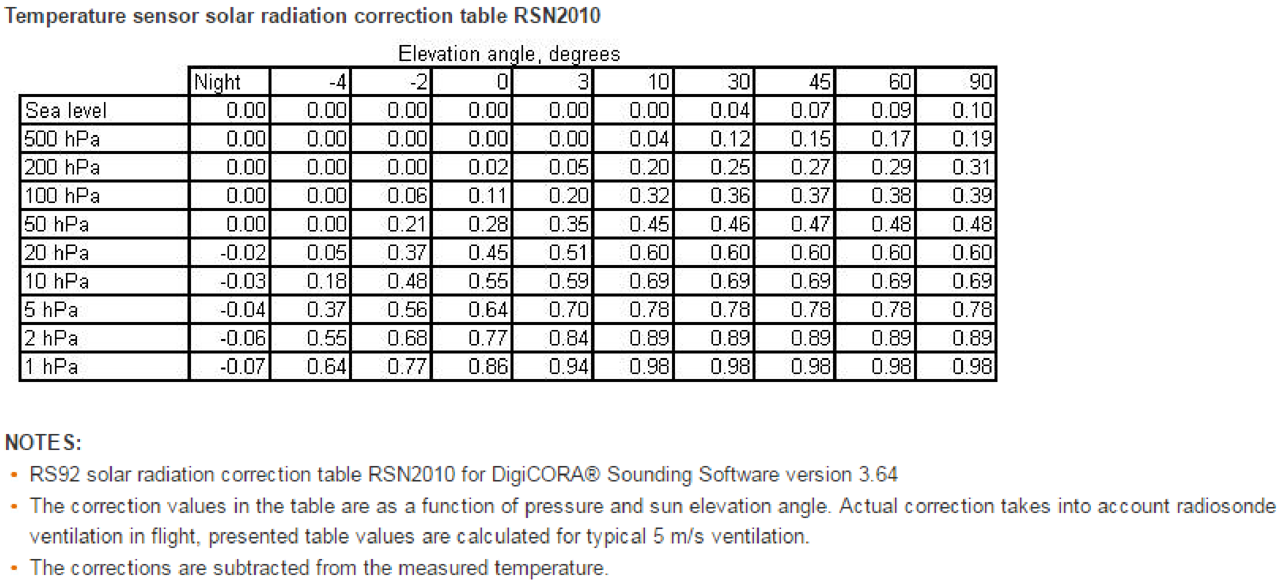
Information / data	Type / value / equation	Notes / description
Name of effect	Radiative dependence of T f(ventilation, pressure)	

Contribution identifier	8a1, $u_{c,RC(\Delta T)}$	
Measurement equation parameter(s) subject to effect	$RH_c = RH_m \frac{p_s(T + f(\frac{\Delta T_{GRUAN} + \Delta T_{Vaisala}}{2}))}{p_s(T)}$ $where\ \Delta T_{GRUAN} = a.\left(\frac{I_a}{p.v}\right)^b$	
Contribution subject to effect (final product or sub-tree intermediate product)	Radiation correction	
Time correlation extent & form	None	Point to point correction
Other (non-time) correlation extent & form	N/A	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	0.5 % RH	Combination of uncertainty from pressure (8a3) and ventilation (8a8) uncertainties.
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …		
Validation		

4.17 Vaisala radiation correction (8a2), $\Delta T_{Vaisala}$

The Vaisala correction for the radiation temperature error is available as a table for various pressures and solar elevation angles [7]. The ascent speed is assumed to be 5 m/s, so does not use the measured values.

There is no separate uncertainty associated with the DigiCora correction in Dirksen et al [1]. However, validation experiments shows a standard deviation of 0.1 K in the troposphere, rising to between 0.3 K and 0.4 K in the stratosphere.



Temperature sensor solar radiation correction table RSN2010

	Elevation angle, degrees									
	Night	-4	-2	0	3	10	30	45	60	90
Sea level	0.00	0.00	0.00	0.00	0.00	0.00	0.04	0.07	0.09	0.10
500 hPa	0.00	0.00	0.00	0.00	0.00	0.04	0.12	0.15	0.17	0.19
200 hPa	0.00	0.00	0.00	0.02	0.05	0.20	0.25	0.27	0.29	0.31
100 hPa	0.00	0.00	0.06	0.11	0.20	0.32	0.36	0.37	0.38	0.39
50 hPa	0.00	0.00	0.21	0.28	0.35	0.45	0.46	0.47	0.48	0.48
20 hPa	-0.02	0.05	0.37	0.45	0.51	0.60	0.60	0.60	0.60	0.60
10 hPa	-0.03	0.18	0.48	0.55	0.59	0.69	0.69	0.69	0.69	0.69
5 hPa	-0.04	0.37	0.56	0.64	0.70	0.78	0.78	0.78	0.78	0.78
2 hPa	-0.06	0.55	0.68	0.77	0.84	0.89	0.89	0.89	0.89	0.89
1 hPa	-0.07	0.64	0.77	0.86	0.94	0.98	0.98	0.98	0.98	0.98

NOTES:

- RS92 solar radiation correction table RSN2010 for DigiCORA® Sounding Software version 3.64
- The correction values in the table are as a function of pressure and sun elevation angle. Actual correction takes into account radiosonde ventilation in flight, presented table values are calculated for typical 5 m/s ventilation.
- The corrections are subtracted from the measured temperature.

Figure 10. DigiCora radiation correction table[8]

Information / data	Type / value / equation	Notes / description
Name of effect	Vaisala radiation correction	
Contribution identifier	8a2, $\Delta T_{\mathrm{Vaisala}}$	
Measurement equation parameter(s) subject to effect	$RH_c = RH_m \dfrac{p_s\left(T + f\left(\dfrac{\Delta T_{GRUAN} + \Delta T_{Vaisala}}{2}\right)\right)}{p_s(T)}$	
Contribution subject to effect (final product or sub-tree intermediate product)	Radiation dry bias correction	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	Up to 4 % RH below the tropopause, 1 % RH above it.	Based on sensitivity tests using change of 0.1 K below the tropopause to 0.4 K above.
Sensitivity coefficient	1	Unused in final calculation.
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …		

Validation	Vaisala validation experiments	

4.18 Pressure (8a3)

The pressure derived from the GRUAN sonde pressure measurement is used in both the GRUAN and Vaisala solar radiation correction models.

The quoted pressure uncertainty is ±0.2 hPa (1σ). When applied to the GRUAN solar correction model the typical temperature uncertainties are <0.001 K (1σ) in the troposphere, rising to ±0.03 K (1σ) in the stratosphere. See the GRUAN pressure product traceability uncertainty document for details of this uncertainty contribution.

Information / data	**Type / value / equation**	**Notes / description**
Name of effect	Pressure	
Contribution identifier	8a3	
Measurement equation parameter(s) subject to effect	Input into both solar radiation correction models	For the GRUAN correction takes form $\Delta T(I_\mathrm{a}, p, v) = a \cdot x^b \quad \text{with } x = \frac{I_\mathrm{a}}{p \cdot v},$
Contribution subject to effect (final product or sub-tree intermediate product)	Radiation dry bias correction	
Time correlation extent & form	Systematic over part of ascent	
Other (non-time) correlation extent & form	Systematic over part of ascent	
Uncertainty PDF shape	Normal & offset	
Uncertainty & units (2σ)	0.0035 % RH below the tropopause and <0.05 % RH above.	Based on sensitivity tests using 0.001 K below the tropopause and 0.03 K above.
Sensitivity coefficient	1	Unused in final calculation.
Correlation(s) between affected parameters	Altitude	
Element/step common for all sites/users?	Yes	
Traceable to …		
Validation		

4.19 Solar Zenith Angle (8a4)

The uncertainty is not considered separately, but is effectively incorporated into the 8a2 Actinic flux radiative transfer model fit uncertainty.

Information / data	Type / value / equation	Notes / description
Name of effect	Solar Zenith Angle	
Contribution identifier	8a4	
Measurement equation parameter(s) subject to effect	-	
Contribution subject to effect (final product or sub-tree intermediate product)	Actinic flux radiative transfer model	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Static	
Uncertainty & units (1σ)	0	
Sensitivity coefficient	1	
Correlation(s) between affected parameters		
Element/step common for all sites/users?		
Traceable to …		
Validation		

4.20 Launch site location (8a5)

The uncertainty is not considered separately.

Information / data	Type / value / equation	Notes / description
Name of effect	Launch site location	
Contribution identifier	8a5	
Measurement equation parameter(s) subject to effect	-	
Contribution subject to effect (final product or sub-tree intermediate product)	SZA	Uses site longitude/latitude & altitude
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Static	

Uncertainty & units (1σ)	0	
Sensitivity coefficient	1	
Correlation(s) between affected parameters		
Element/step common for all sites/users?		
Traceable to …		
Validation		

4.21 Time of launch (8a6)

The uncertainty is not considered separately.

Information / data	Type / value / equation	Notes / description
Name of effect	Time of launch	
Contribution identifier	8a6	
Measurement equation parameter(s) subject to effect	-	
Contribution subject to effect (final product or sub-tree intermediate product)	SZA	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Static	
Uncertainty & units (1σ)	0	
Sensitivity coefficient	1	
Correlation(s) between affected parameters		
Element/step common for all sites/users?		
Traceable to …		
Validation		

4.22 Actinic flux radiative transfer model (8a7)

The dominant systematic error is due to solar radiative heating. Using a heat transfer model, the radiative error for the RS92 temperature sensor was estimated to be approximately 0.5 K at 35 km[9]. This number is comparable to the correction of up to 0.63 K at 5 hPa that was applied by the DigiCora software (prior to version 3.64) in the pro- cessing of RS92 routine soundings until 2010, when this was increased to 0.78 K[10].

The 8th World Meteorological Organization (WMO) radiosonde intercomparison in Yangjiang, China, indicates that the Vaisala-corrected temperature measurements of the RS92 may exhibit a warm bias of up to 0.2 K[11].

A recent comparison between radiosoundings and spaceborne GPS radio occultation measurements reports a 0.5–1K warm bias at 17 hPa for Vaisala-corrected RS92 temperature profiles[12]. The accuracy of the satellite-retrieved temperature is approximately 0.2–0.3K in the middle stratosphere[13,14].

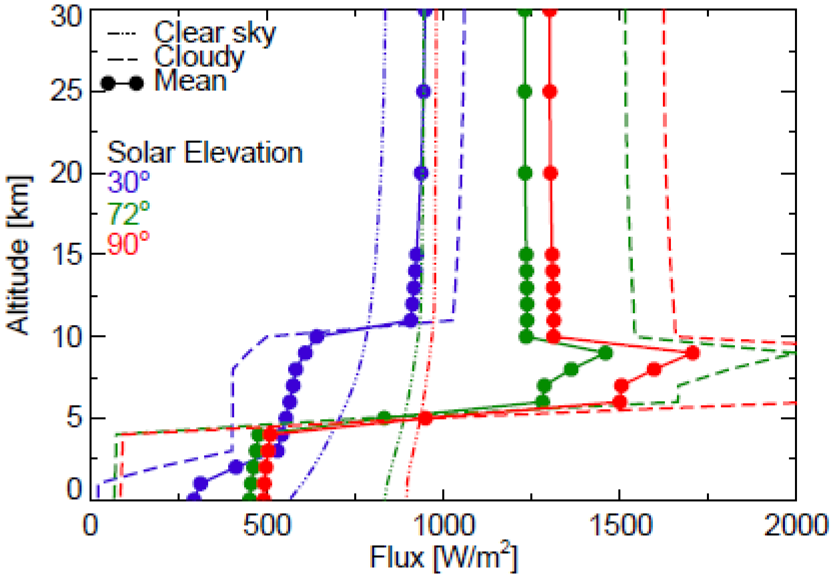


Figure 11. Dirksen figure 5

Information / data	Type / value / equation	Notes / description
Name of effect	Actinic flux model	
Contribution identifier	8a7	
Measurement equation parameter(s) subject to effect	Radiation correction temperature correction $$\Delta T = a.\left(\frac{I_a}{p.v}\right)^b$$	
Contribution subject to effect (final product or sub-tree intermediate product)	Radiation correction	
Time correlation extent & form	Corrected point by point. correlates with time of day (SZA)	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Rectangular	

Uncertainty & units (2σ)	60-250 W/m^2 in the troposphere, 30-200 W/m^2 in the stratosphere dependant on SZA	$u(I_a) = \frac{\lvert I_{a,\text{ cloudy}} - I_{a,\text{ clear sky}}\rvert}{2\sqrt{3}}.$ Low end of range at low SZA, high end of range at high SZA
Sensitivity coefficient	$\Delta T \sim {I_a}^b$	
Correlation(s) between affected parameters	SZA	
Element/step common for all sites/users?	Yes	
Traceable to …		
Validation		

4.23 **Ventilation speed (8a8) u_v & $u_{vent(\Delta T)}$**

The correction of the radiation temperature error also depends on the ventilation speed v. The temperature correction is a function of pressure & ventilation speed, given in Figure 12.

In the GRUAN processing the actual ventilation speed is used, rather than assuming a fixed value. The actual ventilation speed is the sum of the ascent speed, which is derived from the altitude data, plus an additional contribution due to the sonde’s pendulum motion.

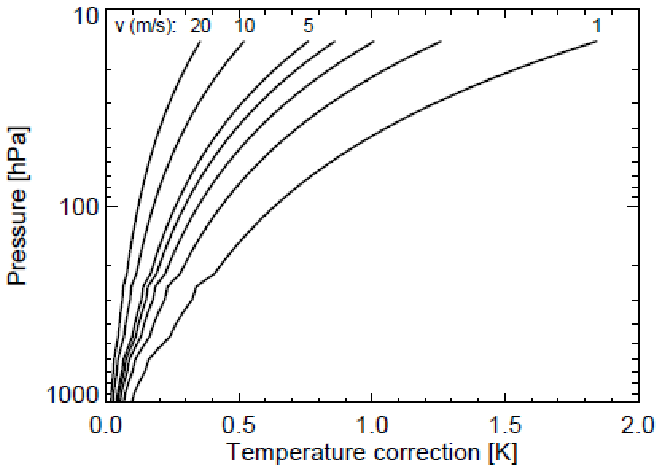


Figure 6. Profiles of the GRUAN radiation temperature correction for ventilation speeds between 1 and 20 m s^{-1}. The correction was calculated for a radiosounding performed in Lindenberg on 17 September 2013 at 12:00 UTC. The kinks in the profiles between 900 and 200 hPa result from the cloud configuration that was used in the Streamer simulations, with cloud layers between 4 and 6 and between 7 and 10 km, which introduces jumps in the simulated radiation profile at the top of the cloud (see the dashed traces in Fig. 5). The maximum solar zenith angle during the sounding was 36.5°.

Figure 12. Ventilation speed temperature correction, from Dirksen et al[1] figure 6

u(v) = ±1m/s (2σ), with the temperature dependence given by:

$$\Delta T \cdot u(v)/v$$

This is equivalent to 0.01 K in the troposphere, rising up to 0.3 K in the stratosphere (2σ).

Information / data	Type / value / equation	Notes / description
Name of effect	Ventilation speed correction	
Contribution identifier	8a8, u_v & $u_{vent(\Delta T)}$	
Measurement equation parameter(s) subject to effect	Relative Humidity	
Contribution subject to effect (final product or sub-tree intermediate product)	Radiation correction (8)	$\Delta T \cdot u(v)/v$
Time correlation extent & form	Systematic	Over ascent
Other (non-time) correlation extent & form	Systematic with Altitude measurement and assumed pendulum motion	Correlated to altitude systematic errors.
Uncertainty PDF shape	Rectangular in velocity, but treated as random in ΔT.	Increase in ventilation speed correction is +1 m.s^{-1} ± 1m.s^{-1} suggesting a defined limit uncertainty.
Uncertainty & units (2σ)	u(v) = ±1m/s (2σ), with the temperature dependence given by $\Delta T \cdot u(v)/v$ Equivalent to 0.2-0.4 % Rh below the tropopause and <0.5 % RH above.	Based on sensitivity tests using 0.01 K (in the trop. upto 0.3 K in the strat (2σ)
Sensitivity coefficient	1	
Correlation(s) between affected parameters	Altitude measurement	
Element/step common for all sites/users?	Yes	
Traceable to …		
Validation		

4.24 Altitude (8a9)

Not considered separately – only uncertainty on derived vertilation speed (8a5).

The altitude product from the GRUAN sondes have a typical uncertainty of ±1 m (1σ) in the troposphere, increasing to ±1.5 m (1σ) in the stratosphere.

Information / data	Type / value / equation	Notes / description

Name of effect	Altitude	
Contribution identifier	8a9	
Measurement equation parameter(s) subject to effect	-	
Contribution subject to effect (final product or sub-tree intermediate product)	Ventilation speed	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	1.5 m	
Sensitivity coefficient	1	Unused in final calculation.
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	No	
Validation	Ventilation speed validation experiments.	

4.25 Sensor orientation (8a10)

Due to the fact that the RS92 temperature sensor is a wire rather than a sphere, the direct solar flux onto the sensor depends on its orientation. The geometry factor g accounts for the reduction of the exposed area of the temperature sensor due to spinning of the radiosonde, which causes the orientation of the sensor wire to cycle between being parallel and perpendicular to the solar rays. Currently, a value of 0.5 is used for g, but this may change in the next version of the GRUAN processing.

Information / data	Type / value / equation	Notes / description
Name of effect	Sensor orientation	
Contribution identifier	8a10	
Measurement equation parameter(s) subject to effect	-	
Contribution subject to effect (final product or sub-tree intermediate product)	Radiation correction	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Static	

Uncertainty & units (1σ)	0	
Sensitivity coefficient	1	
Correlation(s) between affected parameters		
Element/step common for all sites/users?		
Traceable to …		
Validation		

4.26 Cloud configuration (8a11)

No separate contribution – the uncertainty is effectively included as part of the radiative model fit uncertainty (8a1).

Information / data	Type / value / equation	Notes / description
Name of effect	Cloud configuration	
Contribution identifier	8a11	
Measurement equation parameter(s) subject to effect	-	
Contribution subject to effect (final product or sub-tree intermediate product)	Actinic flux Radiative transfer model	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Static	
Uncertainty & units (1σ)	0	
Sensitivity coefficient	1	
Correlation(s) between affected parameters		
Element/step common for all sites/users?		
Traceable to …		
Validation		

4.27 Albedo (8a12) $u_{c, (Ia)}$ & $u_{u, Ia(\Delta T)}$

$$\Delta T \cdot u_{\mathrm{c}}(I_{\mathrm{a}})/I_{\mathrm{a}}$$

where ΔT is the solar radiation correction term and

$$u_c(I_a) = \frac{1}{2\cdot\sqrt{3}}\left|I_a^{\text{clear sky}} - I_a^{\text{cloudy}}\right|$$

Information / data	Type / value / equation	Notes / description
Name of effect	Albedo	
Contribution identifier	8a12	
Measurement equation parameter(s) subject to effect	Radiation correction temperature correction $\Delta T = a.\left(\frac{I_a}{p.v}\right)^b$ Where Albedo is used to determine I_a	
Contribution subject to effect (final product or sub-tree intermediate product)	Radiation correction	
Time correlation extent & form	Corrected point by point. correlates with time of day (SZA)	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Rectangular	
Uncertainty & units (2σ)	0.8 % RH below the tropopause and 0.2 % RH above.	60-250 W/m^2 in the troposphere, 30-200 W/m^2 in the stratosphere dependant on SZA, RH uncertainty found using sensitivity tests using uncertainty in ΔT of <0.05 K (2σ) throughout the ascent.
Sensitivity coefficient	$\Delta T \sim {I_a}^b$	
Correlation(s) between affected parameters	SZA	
Element/step common for all sites/users?	Yes	
Traceable to …		
Validation		

4.28 Radiation sensitivity factor (8b), f

The radiation sensitivity factor, f, accounts for the greater sensitivity of the humidity sensor to radiative heating than the temperature sensor[15]. As a result of changes made to the radiosonde design the sensitivity factor depends on the year of production, different values are shown in table 2.

Table 3 Radiative heating sensitivity factor value and uncertainty for different production years

Production year	Sensitivity factor, f	U(f)
<2006	13	4
2006-2008	10	3
2009-present	6.5	2

Information / data	Type / value / equation	Notes / description
Name of effect	Radiation sensitivity factor	
Contribution identifier	8b, f	
Measurement equation parameter(s) subject to effect	$RH_c = RH_m \frac{p_s(T + f\Delta T)}{p_s(T)}$	
Contribution subject to effect (final product or sub-tree intermediate product)	Radiation dry bias correction	
Time correlation extent & form	Across all sondes within production year ranges.	
Other (non-time) correlation extent & form	Over sounding	
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	$u_c(RC_f) = RH_m \frac{p_{s(T+(f+u(f))\Delta T)-p_S(T+(f-u(f))\Delta T)}}{2 * p_S(T)}$	From 0.5 to 2 % RH below the tropopause and <0.25 % RH above.
Sensitivity coefficient	1	
Correlation(s) between affected parameters	Radiation correction combination.	
Element/step common for all sites/users?	yes	
Traceable to …		
Validation		

4.29 Saturation Vapour Pressure Formula (8c), ps(T)

The radiative dry bias correction uses the Hyland and Wexler formulation of saturation vapour pressure, ps.

$$p_s = \exp[\sum_{i=-1}^{3} h_i T^i + h_4 \ln(T)]$$

Where T is the temperature in kelvin and the coefficients h_i are as shown in table 3.

Table 4 The coefficients used for calculating saturation vapour pressure in the Hyland and Wexler 1983 formulation.

Coefficient	value
h_{-1}	$-0.58002206 \times 10^{4}$
h_0	0.13914993×10^{1}
h_1	$-0.48640239 \times 10^{-1}$
h_2	$0.41764768 \times 10^{-4}$
h_3	$-0.14452093 \times 10^{-7}$
h_4	0.65459673×10^{0}

The uncertainty contribution from using this formulation was determined using sensitivity test with changes in the uncertainty in the radiation correction, calculated as shown in section 4.14 observed for changes in the coefficients. From this it was seen that unless the changes to the coefficients were large enough to affect the fifth significant figure then the changes in the uncertainty of the radiation correction where less than 1% of the overall uncertainty contribution.

Information / data	Type / value / equation	Notes / description
Name of effect	Saturation vapour pressure calculation	
Contribution identifier	8c, ps(T)	
Measurement equation parameter(s) subject to effect	RH = e/ew	
Contribution subject to effect (final product or sub-tree intermediate product)	Radiation dry bias correction	
Time correlation extent & form	Across all soundings	
Other (non-time) correlation extent & form	none	
Uncertainty PDF shape	normal	
Uncertainty & units (1σ)	<0.02 % RH	Assuming the uncertainty in the coefficients only affects beyond the fifth significant figure.
Sensitivity coefficient	1	Unused in final calculation.
Correlation(s) between affected parameters		
Element/step common for all sites/users?	yes	
Traceable to …	Hyland and Wexler 1983	
Validation		

4.30 Time Lag Correction (9), $u_c(TL)$

The response of the humidity sensor slows with decreasing temperature which flattens gradients and smooths structure in the profile. This results from the need for water molecules to diffuse into or out of the sensor[4]. This effect starts to be significant at -40 °C. To correct the time lag the GRUAN processing models it as a low-pass filter with exponential kernel, as shown below:

$$RH_i^m = \frac{\sum_{j=0}^{i} RH_j^a \exp(\frac{t_j - t_i}{\tau_i})}{\sum_{j=0}^{i} \exp(\frac{t_j - t_i}{\tau_i})}$$

Where RH^m is the measured humidity and RH^a is the ambient humidity. Τ is the temperature dependent time constant and t is time. The correction for the time-lag error then follows from inverting this equation to find RH^a:

$$RH_i^{a^*} = RH_i^m + \sum_{j=0}^{i-1} (RH_i^m - RH_i^{a^*}) \exp(\frac{t_j - t_i}{\tau_i})$$

Where RH^{a*} is the corrected ambient humidity.

The correction of the time-lag as described in section 3.29 is applied to the measured RH humidity profile before the low-pass digital filter. The uncertainty here is the correlated uncertainty of the time-lag correction and results from the uncertainty of the time constant, τ.

Information / data	Type / value / equation	Notes / description
Name of effect	Calculate ambient RH using time-lag model	
Contribution identifier	9, RH^{a*}, $u_c(TL)$	
Measurement equation parameter(s) subject to effect	$RH_i^{a^*} = RH_i^m + \sum_{j=0}^{i-1} (RH_i^m - RH_i^{a^*}) \exp(\frac{t_j - t_i}{\tau_i})$	
Contribution subject to effect (final product or sub-tree intermediate product)	Time lag correction	
Time correlation extent & form	Long-term	
Other (non-time) correlation extent & form	Throughout profile	
Uncertainty PDF shape	rectangular	
Uncertainty & units (2σ)	$u_c(TL) = 0.5\|RH(\tau + u(\tau)) - RH(\tau - u(\tau))\|$	Usually <0.5 % RH, peaks at 2 % RH. From Dirksen et al. figure 16, see figure 4.

Sensitivity coefficient	1	
Correlation(s) between affected parameters		
Element/step common for all sites/users?		
Traceable to …		
Validation		

4.31 Time constant (9a), τ

The time constant is used to describe the time lag response and it is the time required for the sensor to respond to 63 % of an instantaneous change in ambient relative humidity. The time constant is related to temperature, T.

$$\tau = A * \exp(c_0 + c_1 * T)$$

With the parameters A = 0.8, c_0 = -0.7399, c_1 = -0.07718. It is assumed that the time constant is the same for increasing and decreasing humidity.

Information / data	Type / value / equation	Notes / description
Name of effect	Time constant	
Contribution identifier	9a, τ	
Measurement equation parameter(s) subject to effect	$RH_i^{a^*} = RH_i^m + \sum_{j=0}^{i-1} \left(RH_i^m - RH_i^{a^*}\right) \exp(\frac{t_j - t_i}{\tau_i})$	
Contribution subject to effect (final product or sub-tree intermediate product)	Time lag correction	
Time correlation extent & form	Long term	
Other (non-time) correlation extent & form	Throughout sounding	
Uncertainty PDF shape		
Uncertainty & units (2σ)	$u(\tau) = 0.5 * \tau(1 - A) \approx 0.1\tau$ or 1.5-3 s	
Sensitivity coefficient	unspecified	
Correlation(s) between affected parameters	Calibration correction factor	Both depend on temperature.
Element/step common for all sites/users?	Yes	

Traceable to …		
Validation		

4.32 Low pass digital filter with cut-off (10), fc

The correction used for the time-lag error also amplifies noise in the profile. This is removed using a low pass digital filter. The cut-off for the filter, $f_c=3/\tau$ and is less than 0.1 Hz. The factor of 3 is to prevent the removal of genuine structures in the profile when τ is large.

The uncertainty is the statistical noise calculated as part of the smoothing step. This is calculated as:

$$u(\overline{s_i}) = \sqrt{\frac{N'}{N'-1}\sum_{j=-M}^{M} c_j^2 (s_{i+j} - \overline{s_i})^2}$$

Where s is the smoothed data point an N' corresponds to the width of the Gaussian-shaped kernel function.

Information / data	Type / value / equation	Notes / description
Name of effect	Low pass digital filter	
Contribution identifier	10, U_u(RH)	
Measurement equation parameter(s) subject to effect	Relative humidity	
Contribution subject to effect (final product or sub-tree intermediate product)	Time lag correction	
Time correlation extent & form	none	
Other (non-time) correlation extent & form	50 points up and down profile	Uses a sample of 100 points.
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	0.5 – 2 % RH	From Dirksen et al. figure 16, see figure 4.
Sensitivity coefficient	1	
Correlation(s) between affected parameters		
Element/step common for all sites/users?		
Traceable to …		
Validation		

4.33 Corrected RH values with associated uncertainties (11)

The total uncertainty of the corrected relative humidity profile is the sum in quadrature of the calibration, dry bias correction, radiative heating correction, time lag correction and statistical uncertainties.

Information / data	Type / value / equation	Notes / description
Name of effect	Corrected RH values with associated uncertainties.	
Contribution identifier	11,u(RH)	
Measurement equation parameter(s) subject to effect	Relative Humidity	
Contribution subject to effect (final product or sub-tree intermediate product)	Relative Humidity	
Time correlation extent & form	none	
Other (non-time) correlation extent & form	>10s, usually <40s	Varies according to low pass digital filter, available as res_rh.
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	$u(RH) = \sqrt{u_c(cal)^2 + u_c(cc)^2 + u_c(TL)^2 + u_c(RC)^2 + u_u(RH)^2}$	6 % RH
Sensitivity coefficient	1	
Correlation(s) between affected parameters	none	
Element/step common for all sites/users?	Yes	
Traceable to …		
Validation		

5 Uncertainty Summary

Element identifier	Contribution name	Uncertainty contribution form	Typical value	Traceability level (L/M/H)	Random, structured random, quasi-systematic or systematic ?	Correlated to
1	Thin film capacitor heated twin sensor	constant	0	H	random	none
2, u_c	Calibrated in Vaisala CAL4 facility	constant	2 % RH	H	systematic	4
2a	Reference humidity sensors	constant	0.8-1.2 % RH	H	systematic	
3	Transported and stored at launch site	constant	0	L	systematic	none
4, u_c(cal)	Pre-flight ground check re-calibration	$\sqrt{u_c^2 + u_{c,GC25}^2 + u_{c,absolute\ SHC}^2 + u_{c,relative}^2(Cal)RH}$	1-3 % RH	H	Quasi-systematic	10
4a, $u_{c,GC25}$	Ground check over desiccant	$\sqrt{(\frac{\Delta U_1}{3})^2 + (\frac{\Delta U_2}{3})^2 + (U_1 - U_2)_{GC25}^2}$	<1 % RH	H	Quasi-systematic	4
4b, $u_{c,absolute\ SHC}$	Ground check in standard humidity chamber	$\sqrt{(U_1 - U_2)_{SHC}^2}$		H	Quasi-systematic	4, 4c
4c, $u_{c,relative}$(cal)	Relative calibration uncertainty	$\sqrt{(U_1 - U_{SHC})^2 + (U_2 - U_{SHC})^2} / U_{SHC}$	0.028* RH	H	Quasi-systematic	4, 4b
5	Sonde measurements every second during ascent	Statistical uncertainty	0.05-0.1 % RH		random	None
6	Data transmitted to ground station	constant	0	L	systematic	None
7, u_c(cc)	Calibration correction	$\frac{u(f_{cc})}{f_{cc}} RH^*$	0.5 – 4 % RH		systematic	10

	of temperature dependant bias					
7a	Temperature	See temperature PTU documents				7b,9a2
7b	Calibration correction factor	Constant, interpolated between reference temps	0.01-0.1		systematic	7
8, $u_c(RC)$	Radiation dry bias correction	$\sqrt{u_c(RC_f)^2+u_c(RC_t)^2}$	5 % RH	M		10
8a, $u_c(RC_T)$	Radiative correction combination	$RH_m\frac{p_s\left(T+f\left(\Delta T+u(\Delta T)\right)\right)-p_s\left(T+f\left(\Delta T-u(\Delta T)\right)\right)}{2*p_s(T)}$	4 % RH	M	Systematic	8
8a1	Radiative dependence of T reading as a function of ventilation and pressure	constant	0.5 % RH	M	systematic	none
8a2	Vaisala solar radiation correction	constant	1 - 4 % RH	M	systematic	8a1
8a3	Pressure	constant	<0.05 % RH	M	Rand	Press PTU, 8a10
8a4	Solar zenith angle	Constant	0	M	Systematic (over ascent)	
8a5	Launch site location	Constant	0	H	Systematic	
8a6	Time of launch	constant	0	H	Systematic (over ascent)	
8a7, $u(I_a)$	Actinic flux radiative transfer model	$\frac{\lvert I_{a,cloudy}-I_{a,clear\ sky}\rvert}{2\sqrt{3}}$	<350 Wm^{-2}	M	Quasi-systematic	Altitude
8a8, $u_{u,vent}(\Delta T)$	Ventilation speed	$\Delta T(\frac{u(v)}{v})$	<0.5 % RH	M	Quasi-systematic	Altitude
8a9	Altitude	Constant	0	M	Quasi-systematic	Altitude PTU
8a10	Sensor orientation	constant	0	L	systematic	8a1
8a11	Cloud	constant	0	L	systematic	

	configuration					
8a12	Albedo	$\Delta T \frac{u_c(I_a)}{I_a}$	<0.8% RH	M	systematic	None
8b	Radiation sensitivity factor $u_c(RC_f)$	$\frac{p_{s(T+(f+u(f))\Delta T)-p_s(T+(f-u(f))\Delta T)}}{2 * p_s(T)}$	0.5 – 2 %	M	Systematic	
8c	Saturation vapour pressure	constant	<0.02 % RH	L	Systematic	None
9, u_c(TL)	Calculate ambient RH using time-lag model	$0.5 \lvert RH(\tau + u(\tau)) - RH(\tau - u(\tau)) \rvert$	1-2 % RH	M	Systematic	9a
9a, u(τ)	Time constant	$0.5 * \tau(1 - A)$		M	Sytematic	7a
10	Low pass digital filter	Statistical uncertainty	0.5 – 2 % RH	M	Random	9a
11, u(RH)	Corrected RH values	$\sqrt{u_c(cal)^2 + u_c(cc)^2 + u_c(TL)^2 + u_c(RC)^2 + u_u(R}$	6 % RH	M		

The total uncertainty in the GRUAN RS92 relative humidity product is the sum in quadrature of the uncertainties from the statistical uncertainty, calibration and the different corrections applied. This is shown in equation 1 below.

$$u(RH) = \sqrt{u_c(cal)^2 + u_c(cc)^2 + u_c(TL)^2 + u_c(RC)^2 + u_u(RH)^2} \qquad (1)$$

Where u_c(cal) is the uncertainty in calibration, u_c(cc) is the uncertainty in the calibration correction, u_c(TL) is the uncertainty in the time lag correction, u_c(RC) is the uncertainty in the radiative dry bias correction.

The total uncertainty in relative humidity, u(RH), is usually 6 % RH, but can peak above 10 % RH, and drops to between 2 and 2.5 % RH in the upper part of the profile, above the tropopause. However relative uncertainty is larger in the upper part of the profile because of how low the relative humidity measurements are. The total uncertainty takes into account four sources of correlated uncertainty and one source of statistical uncertainty. The statistical uncertainty, u_u(RH), is greatest below the tropopause and is usually below 5 % RH. Above the tropopause it is usually below 2 % RH. With the exception of narrow peaks in the statistical uncertainty, the correlated uncertainty contributes more to the total uncertainty throughout the profile. This include the calibration uncertainty, u_c(cal), which is itself a combination of manufacturer calibration uncertainty and ground check re-calibration uncertainty is between 2 and 3 % RH throughout most of the profile but is larger near the surface as a result of the relative uncertainty determined from the standard humidity chamber. The uncertainty contribution of the calibration dry bias correction, u_c(cc), increases from about 1.5 % RH near the surface to up to 5 % RH at the tropopause. Above this level u_c(cc) drops to below 0.5 % RH. The uncertainty contribution from the radiative heating correction, u_c(RC), starts below 2 % RH and rises to above 5 % RH near the tropopause. in soundings where it is present this is the largest contribution to the correlated uncertainty. The last contribution to the correlated uncertainty is from the time-lag correction, u_c(TL), is the smallest contributor to the correlated uncertainty and is usually below 2 %

RH. Three of the contributions to the correlated uncertainty are temperature related and correlated uncertainty peaks near the tropopause, where the temperature is low but there is still fairly high atmospheric RH. Most of the total uncertainty is correlated uncertainty.

5.1 Traceability uncertainty analysis

Traceability level definition is given in Table 5.

Table 5. Traceability level definition table

Traceability Level	Descriptor	Multiplier
High	SI traceable or globally recognised community standard	1
Medium	Developmental community standard or peer-reviewed uncertainty assessment	3
Low	Approximate estimation	10

Analysis of the summary table would suggest the following contributions, shown in Table 6, should be considered further to improve the overall uncertainty of the GRUAN temperature product. The entries are given in an estimated priority order.

Table 6. Traceability level definition further action table.

Element identifier	Contribution name	Uncertainty contribution form	Typical value	Traceability level (L/M/H)	Random, structured random, quasi-systematic or systematic?	Correlated to
8c	Saturation vapour pressure	constant	<0.02 % RH	L	Systematic	None
8a8, $u_{u,vent}(\Delta T)$	Ventilation speed	$\Delta T(\frac{u(v)}{v})$	<0.5 % RH	M	Quasi-systematic	Altitude
8a4	Solar zenith angle	Constant	0	M	Systematic (over ascent)	
8a5	Launch site location	Constant	0	H	Systematic	
8a6	Time of launch	constant	0	H	Systematic (over ascent)	
8a7, $u(I_a)$	Actinic flux radiative transfer model	$\frac{\lvert I_{a,cloudy} - I_{a,clear\ sky}\rvert}{2\sqrt{3}}$	<350 Wm^{-2}	M	Quasi-systematic	Altitude
8a9	Altitude	Constant	0	M	Quasi-	Altitude

					systematic	PTU
8a10	Sensor orientation	constant	0	L	systematic	8a1
8a11	Cloud configuration	constant	0	L	systematic	

5.2 Recommendations

An assessment of the Vaisala correction for radiative heating uncertainty should be evaluated, as currently the uncertainty is only calculated for the GRUAN correction and sensitivity tests indicate it may have a significant contribution.

It would also be useful for the ground-check information to be included in the data files, particularly as this influences whether calibration uncertainty is calculated from the ground check or just included assumed.

More detail about the saturation vapour pressure formula could be given in the documentation, since although Hyland and Wexler 1983 is widely referenced it can be hard to find.

There are contributions that do not have an assigned uncertainty. Some analysis to determine the magnitude of these potential contributions would better constrain the uncertainty budget.

Some contributions are discussed, but not used in the overall uncertainty calculation, e.g. uncertainty from the temperature product. The uncertainty contribution from these elements should be quantified and used.

6 Conclusions

The GRUAN RS92 radiosonde humidity product has been assessed against the GAIA CLIM traceability and uncertainty criteria.

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Product Traceability and Uncertainty for the GRUAN RS92 radiosonde geopotential height product

Version 2.0

GAIA-CLIM
Gap Analysis for Integrated
Atmospheric ECV Climate Monitoring
Mar 2015 - Feb 2018

A Horizon 2020 project; Grant agreement: 640276

Date: 30 November 2017

Dissemination level: PU

Work Package 2; Complied by David Medland, Paul Green & Tom Gardiner (NPL)

Table of Contents

Version history

Version	Principal updates	Owner	Date
1.0	First issue	NPL	26.07.2017
2.0	Issued as annex D to D2.6	NPL	30.11.2017

1 Product overview

Product name: In-situ radiosonde RS92 geopotential height
Product technique: Capacitive pressure sensor / GPS altitude
Product measurand: Pressure/Altitude
Product form/range: profile (ground to 30km, 1sec sampling)
Product dataset: GRUAN Reference level sonde dataset
Site/Sites/Network location:

SITE	LAT	LON	HEIGHT(m)	LOCATION	COUNTRY
BEL	39.05	-76.88	53	Beltsville	US
BOU	71.32	-156.61	8	Boulder	US
CAB	51.97	4.92	1	Cabauw	NL
LAU	-45.05	169.68	370	Lauder	NZ
LIN	52.21	14.12	98	Lindenberg	DE
NYA	78.92	11.92	5	Ny-Ålesund	NO
PAY	46.81	6.95	491	Payerne	CH
POT	40.60	15.72	720	Potenza	IT
SOD	67.37	26.63	179	Sodankylä	FI

Product time period: 20 May 2006 to present
Data provider: Site operators, see www.gruan.org
Instrument provider: See www.gruan.org
Product assessor: David Medland, NPL
Assessor contact email: david.medland@npl.co.uk

1.1 Guidance notes

For general guidance see the Guide to Uncertainty in Measurement & its Nomenclature, published as part of the GAIA-CLIM project.

This document is a measurement product technical document which should be stand-alone i.e. intelligible in isolation. Reference to external sources (preferably peer-reviewed) and documentation from previous studies is clearly expected and welcomed, but with sufficient explanatory content in the GAIA-CLIM document not to necessitate the reading of all these reference documents to gain a clear understanding of the GAIA-CLIM product and associated uncertainties entered into the Virtual Observatory (VO).

In developing this guidance, we have created a convention for the traceability identifier numbering as shown in Figure 1. The 'main chain' from raw measurand to final product forms the axis of the diagram, with top level identifiers (i.e. 1, 2, 3 etc.). Side branch processes add sub-levels components to the top level identifier (for example, by adding alternate letters & numbers, or 1.3.2 style nomenclature).

The key purpose of this sub-level system is that all the uncertainties from a sub-level are summed in the next level up.

For instance, using Figure 1, contributors 2a1, 2a2 and 2a3 are all assessed as separate components to the overall traceability chain (have a contribution table). The contribution table for (and uncertainty associated with) 2a, should combine all the sub-level uncertainties (and any additional uncertainty intrinsic to step 2a). In turn, the contribution table for contributor 2, should include all uncertainties in its sub-levels.

Therefore, only the top level identifiers (1, 2, 3, etc.) shown in bold in the summary table need be combined to produce the overall product uncertainty. The branches can therefore be considered in isolation, for the more complex traceability chains, with the top level contribution table transferred to the main chain. For instance, see Figure 2 & Figure 3 as an example of how the chain can be divided into a number of diagrams for clearer representation.

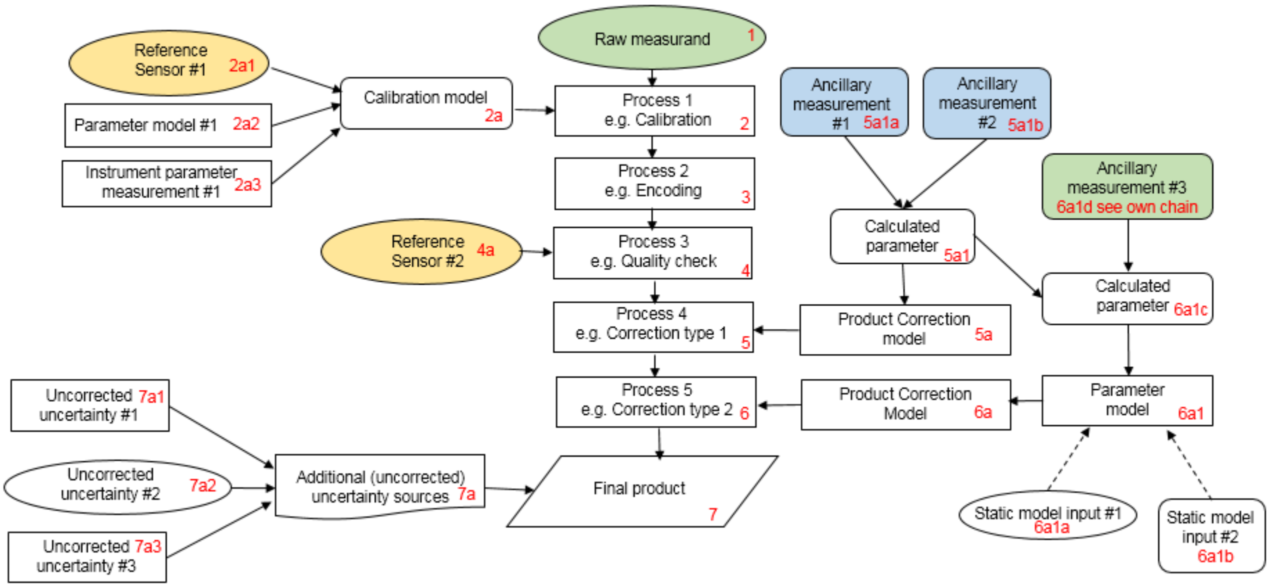


Figure 1. Example traceability chain. Green represents a key measurand or ancillary measurand recorded at the same time with the product raw measurand. Yellow represents a source of traceability. Blue represents a static ancillary measurement

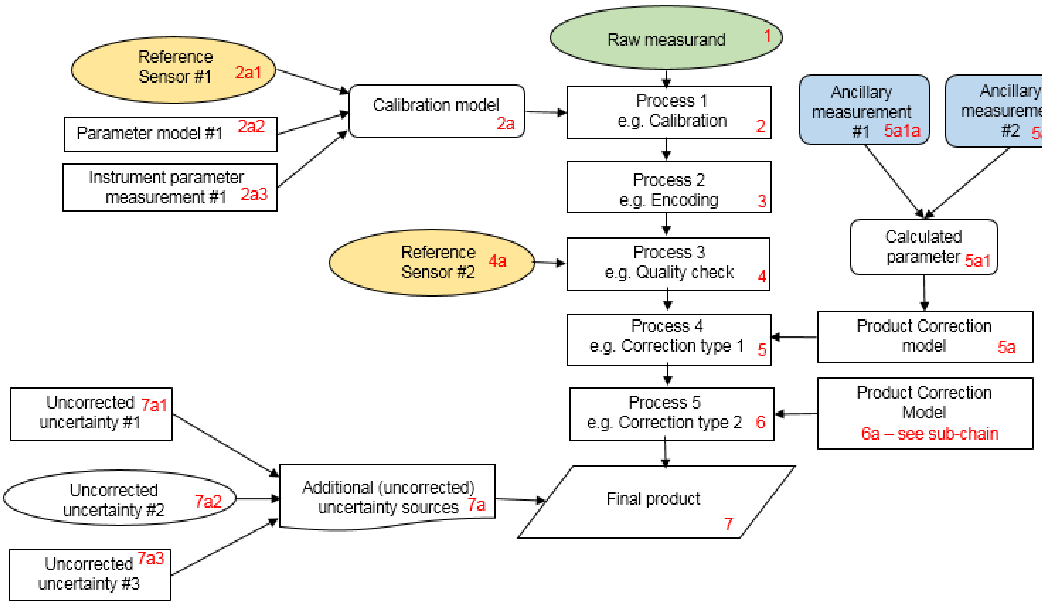


Figure 2. Example chain as sub-divided chain. Green represents a key measurand or ancillary measurand recorded at the same time with the product raw measurand. Yellow represents a source of traceability. Blue represents a static ancillary measurement

When deciding where to create an additional sub-level, the most appropriate points to combine the uncertainties of sub-contributions should be considered, with additional sub-levels used to illustrate where their contributions are currently combined in the described process.

A short note on colour coding. Colour coding can/should be used to aid understanding of the key contributors, but we are not suggesting a rigid framework at this time. In Figure 1, green represents a key measurand or ancillary or complementary measurand recorded at the same time with the raw measurand; yellow represents a primary source of traceability & blue represents a static ancillary measurement (site location, for instance). Any colour coding convention you use, should be clearly described.

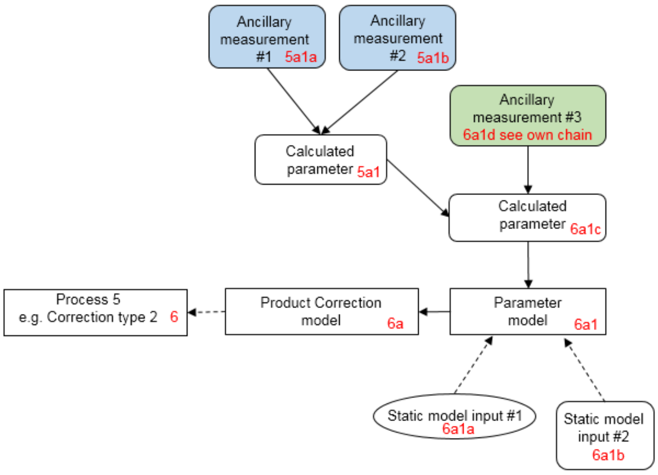


Figure 3. Example chain contribution 6a sub-chain. Green represents a key measurand or ancillary measurand recorded at the same time with the product raw measurand. Blue represents a static ancillary measurement

The contribution table to be filled for each traceability contributor has the form seen in Table 1.

Table 1. The contributor table.

Information / data	Type / value / equation	Notes / description
Name of effect		
Contribution identifier		
Measurement equation parameter(s) subject to effect		
Contribution subject to effect (final product or sub-tree intermediate product)		
Time correlation extent & form		
Other (non-time) correlation extent & form		
Uncertainty PDF shape		
Uncertainty & units		
Sensitivity coefficient		
Correlation(s) between affected parameters		

Element/step common for all sites/users?		
Traceable to …		
Validation		

Name of effect – The name of the contribution. Should be clear, unique and match the description in the traceability diagram.

Contribution identifier - Unique identifier to allow reference in the traceability chains.

Measurement equation parameter(s) subject to effect – The part of the measurement equation influenced by this contribution. Ideally, the equation into which the element contributes.

Contribution subject to effect – The top level measurement contribution affected by this contribution. This can be the main product (if on the main chain), or potentially the root of a side branch contribution. It will depend on how the chain has been sub-divided.

Time correlation extent & form – The form & extent of any correlation this contribution has in time.

Other (non-time) correlation extent & form – The form & extent of any correlation this contribution has in a non-time domain. For example, spatial or spectral.

Uncertainty PDF shape – The probability distribution shape of the contribution, Gaussian/Normal Rectangular, U-shaped, log-normal or other. If the form is not known, a written description is sufficient.

Uncertainty & units – The uncertainty value, including units and confidence interval. This can be a simple equation, but should contain typical values.

Sensitivity coefficient – Coefficient multiplied by the uncertainty when applied to the measurement equation.

Correlation(s) between affected parameters – Any correlation between the parameters affected by this specific contribution. If this element links to the main chain by multiple paths within the traceability chain, it should be described here. For instance, SZA or surface pressure may be used separately in a number of models & correction terms that are applied to the product at different points in the processing. See Figure 1, contribution 5a1, for an example.

Element/step common for all sites/users – Is there any site-to-site/user-to-user variation in the application of this contribution?

Traceable to – Describe any traceability back towards a primary/community reference.

Validation – Any validation activities that have been performed for this element?

The summary table, explanatory notes and referenced material in the traceability chain should occupy <= 1 page for each element entry. Once the summary tables have been completed for the full end-to-end process, the uncertainties can be combined, allowing assessment of the combined uncertainty, relative importance of the contributors and correlation scales both temporally and spatially. The unified form of this technical document should then allow easy comparison of techniques and methods.

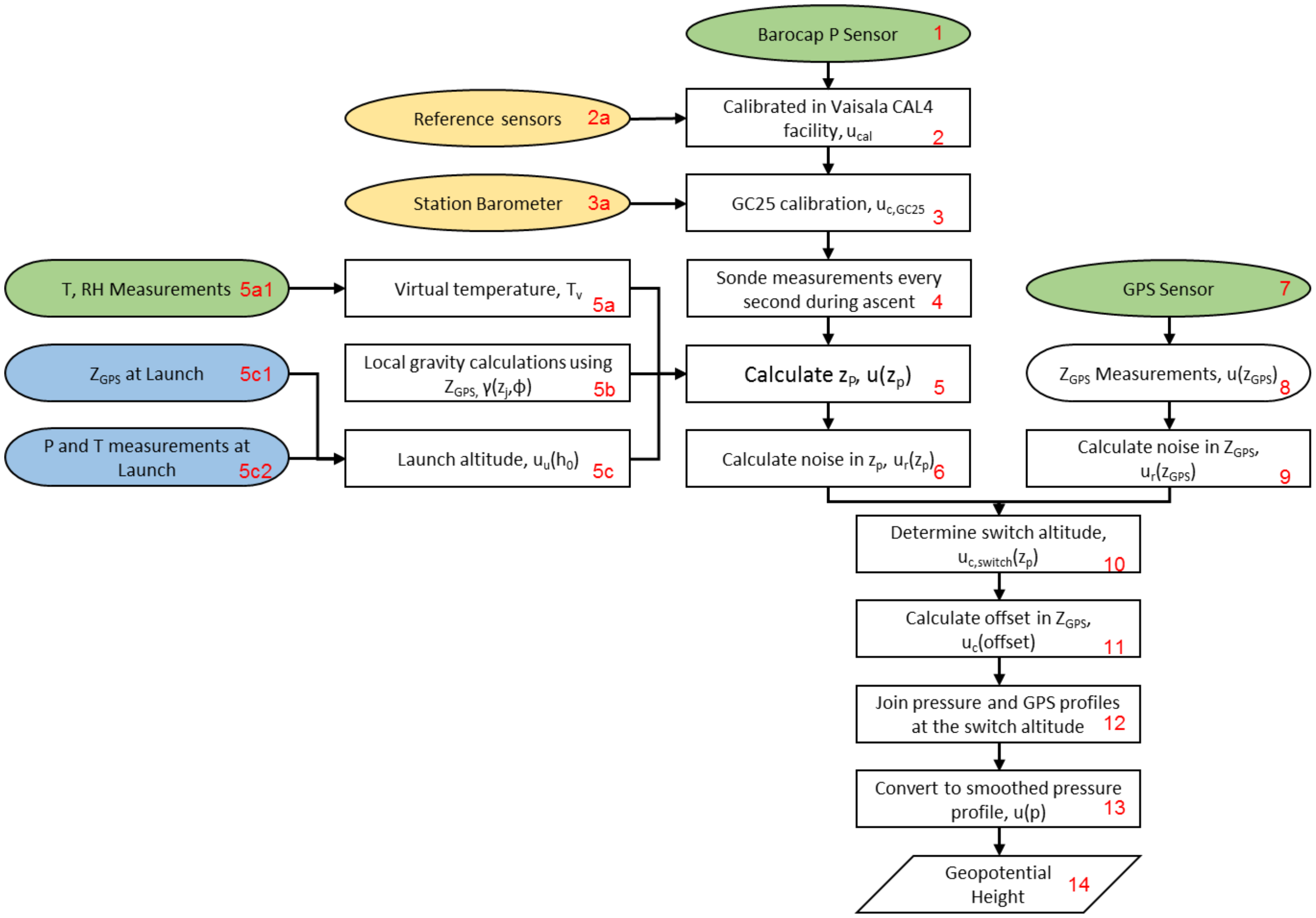
2 Introduction

This document describes the product traceability and uncertainty information for the GRUAN (GCOS (Global Climate Observing System) Reference Upper-Air Network) RS92 radiosonde geopotential height product. The derivation of the geopotential height uses the GRUAN RS92 radiosonde altitude product as well as the GRUAN RS92 radiosonde pressure product and so the traceability and uncertainty information of these data products is also contained within this document.

The RS92 Radiosonde is equipped with a Barocap, which determines pressure from the capacitance between an electrode on a silicon membrane separated from another electrode by a vacuum. Data is transmitted at 1 second intervals and stored by DigiCora ground station equipment. It is also equipped with a GPS receiver which collects xyz coordinates in WGS-84 (World Geodetic System 1984). These are converted to longitude, latitude and altitude by the DigiCora system using altitude derived from pressure measurements as a reference. Geopotential height is calculated using measurements collected from both of these instruments. The Barocap is calibrated by Vaisala using their CAL4 facility and is recalibrated during a pre-flight ground check using a GC25 unit.

The process through which the GRUAN geopotential height product is derived from raw pressure and altitude data, as well as the methods used at ground check to calibrate the instruments and determine the uncertainty of the data product are described in Dirksen et al[1]. 2014, which has been used for the creation of this document, and the methods and uncertainties detailed here are as they present. The data product was developed to meet the criteria for reference measurements, these include the collection of metadata, the use of well documented algorithms and estimates of the measurement uncertainty. Overall GRUAN uncertainty estimates are 0.6 hPa for pressure and 10-50 m for altitude and geopotential height.

3 Product Traceability Chain



4 Element Contributions

4.1 Barocap pressure sensor (1)

The RS92 radiosonde measures pressure using a Barocap. This has one electrode on a silicon base and another on a silicon membrane separated by a vacuum. As pressure changes so does the separation of the electrodes, varying the capacitance which is converted to a pressure measurement. The uncertainty expressed here is the standard deviation between twin soundings as determined by Vaisala, but is not used in the GRUAN processing.

Information / data	Type / value / equation	Notes / description
Name of effect	Barocap pressure sensor	Random noise of barocap pressure sensor and calibration uncertainty
Contribution identifier	1	
Measurement equation parameter(s) subject to effect	Geopotential height	
Contribution subject to effect (final product or sub-tree intermediate product)	Geometric pressure altitude, pressure readings with uncertainties	
Time correlation extent & form	none	
Other (non-time) correlation extent & form	none	
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	0.5 hPa > 100 hPa 0.3 hPa < 100 hPa	Variability between twin soundings. 2σ. From Vaisala RS92 technical data[2].
Sensitivity coefficient	1	Uncertainty not included in GRUAN processing
Correlation(s) between affected parameters	Launch height uncertainty.	
Element/step common for all sites/users?	yes	
Traceable to …	Vaisala	
Validation	N/A	

4.2 Calibrated in Vaisala CAL4 facility (2), u_{cal}

The uncertainty represented here is the repeatability in calibration which is carried out at Vaisala's CAL-4 facility. This tests the RS92 barocap in 4 chambers with constant temperature and pressure between 1080 and 2 hPa. Ten pressure levels are used to fit a calibration curve at +25 °C and the temperature dependence of the barocap determined by the deviation from this calibration curve.

Information / data	Type / value / equation	Notes / description

Name of effect	Calibrated in Vaisala CAL4 facility.	
Contribution identifier	2, u_{cal}	
Measurement equation parameter(s) subject to effect	Geopotential height	
Contribution subject to effect (final product or sub-tree intermediate product)	Geopotential height	
Time correlation extent & form	Long term	Between calibrations of the reference sensors.
Other (non-time) correlation extent & form	Over flight.	Used in calculating uncertainty in pressure.
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	0.4 hPa >100 hPa 0.3 hPa <100 hPa	Repeatability in calibration. k = 2. From Vaisala RS92 technical data[2].
Sensitivity coefficient	1	
Correlation(s) between affected parameters	Barocap pressure sensors	
Element/step common for all sites/users?	yes	
Traceable to …	Vaisala	
Validation	N/A	

4.3 Reference pressure sensors (2a)

The CAL4 contains PTU reference sensors that are recalibrated at regular intervals against standards that are traceable to NIST for pressure. The operating range and accuracy of the PTU sensors for pressure is 2 (±0.3) to 1080 (±0.3) hPa.

Information / data	**Type / value / equation**	**Notes / description**
Name of effect	Reference pressure sensors	
Contribution identifier	2a	
Measurement equation parameter(s) subject to effect	Geopotential height,	
Contribution subject to effect (final product or sub-tree intermediate product)	Calibrated in Vaisala CAL4 facility	
Time correlation extent & form	Long-term	Correlated over period of reference sensor recalibration, 6 months for digital barometers, 12 months for analogue pressure transmitters[3].

Other (non-time) correlation extent & form	none	
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	<0.3 hPa	K=2, From vaisala 2007 CAL4 technical note[3].
Sensitivity coefficient	1	
Correlation(s) between affected parameters	none	
Element/step common for all sites/users?	yes	
Traceable to …	NIST	
Validation	None	

4.4 GC25 Calibration (3), $u_{c,GC25}$

Determined from the calibration uncertainty of the pressure sensor and the difference between the station barometer and RS92 pressure sensor during ground check. This uses a Vaisala GC25 unit. For the ground check of the pressure sensor a separate reference measurement is used, in this case from the station barometer. This is entered into the GC25 which applies the correction factor, calculated as $c = p_{station}/p_{RS92,GC25}$, which is applied to the entire pressure profile. The GRUAN processing uses the recalibrated data. The uncertainty in the calibration is the geometric sum of the Vaisala calibration uncertainty and a contribution from the applied correction based on the difference in the radiosonde and station barometer pressure readings, this is usually around 0.5 hPa and any sondes with a difference greater than 1.5 hPa are rejected.

Information / data	**Type / value / equation**	**Notes / description**
Name of effect	GC25 Calibration	Pre-launch re-calibration with onsite barometer
Contribution identifier	3, $u_{c,GC25}$	
Measurement equation parameter(s) subject to effect	Geopotential height	
Contribution subject to effect (final product or sub-tree intermediate product)	Geopotential height	
Time correlation extent & form	Long term	Between recalibrations of the station barometer.
Other (non-time) correlation extent & form	Systematic over flight	Does not affect the uncertainty of geopotential height
Uncertainty PDF shape	rectangular	
Uncertainty & units (2σ)	$u_{c,GC25}(p) = \sqrt{u_{cal}^2 + (\frac{\Delta p_{GC25}}{3})^2}$ Using typical values of u_{cal}=0.4 hPa and Δp_{GC25}=0.5 hPa gives $u_{c,GC25}(p)$=0.43 hPa.	U_{cal} is the calibration uncertainty of the pressure sensor. Δp_{GC25} is pressure difference between the sonde and station barometer at

		ground check[1].
Sensitivity coefficient	1	
Correlation(s) between affected parameters	none	
Element/step common for all sites/users?	Yes	
Traceable to …	Barocap pressure sensor, station barometer	
Validation	N/A	

4.5 Station barometer (3a)

The station barometer is used in determining the launch altitude of the sonde and in re-calibrating the sondes pressure sensor.

Information / data	Type / value / equation	Notes / description
Name of effect	Station Barometer	
Contribution identifier	3a	
Measurement equation parameter(s) subject to effect	Geopotential height, Pressure	
Contribution subject to effect (final product or sub-tree intermediate product)	GC25 Calibration	
Time correlation extent & form	Long term systematic	Between re-calibrations of the station barometer
Other (non-time) correlation extent & form	none	
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	< 0.5 m <0.06 hPa	$U_{u,launch}(z_p)$ is included in $u_u(h_0)$ so has to be smaller. Converted to pressure using equation 22 in Dirksen et Al.
Sensitivity coefficient	1	
Correlation(s) between affected parameters	Launch altitude uncertainty	
Element/step common for all sites/users?	yes	
Traceable to …	Station specific	
Validation	N/A	

4.6 Sonde Measurements every second during ascent (4)

The pressure measurements are taken by the radiosonde using the barocap every second after launch during the ascent. The uncorrelated uncertainty associated with this step is calculated as part of step 6, calculate noise in z_p.

Information / data	Type / value / equation	Notes / description
Name of effect	Sonde measurements every second during ascent	
Contribution identifier	4	
Measurement equation parameter(s) subject to effect	Geopotential height, Pressure	
Contribution subject to effect (final product or sub-tree intermediate product)	Geopotential height	
Time correlation extent & form	none	
Other (non-time) correlation extent & form	none	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	0	Covered in element 6
Sensitivity coefficient	1	
Correlation(s) between affected parameters	Virtual temperature	
Element/step common for all sites/users?	yes	
Traceable to …	Vaisala	
Validation	N/A	

4.7 Calculate geometric pressure altitude (5), z_p

The change in geometric altitude between two measurements is calculated from pressure using:

$$\Delta H_{1,2} = \frac{R_d}{\gamma(z_j,\varphi)}\bar{T}_v ln(\frac{p_1}{p_2})$$

Where $\bar{T}_v$ is the average virtual temperature between pressure levels p_1 and p_2, discussed in section 3.8, and $\gamma(z_j,\varphi)$ is the local gravity, discussed in section 3.10. The geometric altitude is then calculated as:

$$z_p = h_0 + \sum \Delta H$$

Where h_0 is the launch altitude. The uncertainty in geometric pressure altitude is calculated as the geometric sum of the random ($u_r(z_p)$, see section 3.14) and correlated uncertainty and the uncertainty in launch height ($u_u(h_0)$, see section 3.11). This uncertainty is dominated by correlated uncertainty which is calculated from the bias of the pressure sensor ΔP:

$$\Delta p = p\,[\exp\left(\frac{\gamma \Delta z}{R_d T}\right) - 1]$$

Where $\Delta z = z_p - z_{GPS}$. The correlated uncertainty $u_c(z_p)$ is then:

$$u_c(z_p) = 0.5 \times (z(p + \Delta p) - z(p - \Delta p))$$

Information / data	Type / value / equation	Notes / description
Name of effect	Geometric pressure altitude	
Contribution identifier	5, z_p	
Measurement equation parameter(s) subject to effect	Geopotential height	
Contribution subject to effect (final product or sub-tree intermediate product)	Geopotential height	
Time correlation extent & form	none	
Other (non-time) correlation extent & form	Sounding, throughout flight	Influences uncertainty in geometric GPS altitude
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	$u(z_p) = \sqrt{u_u(h_0)^2 + u_r(z_p)^2 + u_c(z_p)^2}$	Usually starts at 0.5 m and increases with altitude up to between 10-50 m. the uncorrelated uncertainty is usually <2 m[1].
Sensitivity coefficient	1	
Correlation(s) between affected parameters	none	
Element/step common for all sites/users?	yes	
Traceable to …	Launch altitude uncertainty, bias of pressure sensor	
Validation	Altitude from GPS	

4.8 Virtual temperature (5a), T_v

Virtual temperature of a moist air parcel is equal to the temperature that a dry air parcel of the same pressure and density would have. It is used in calculating geometric altitude from pressure, or pressure from geometric altitude, which depends on the average virtual temperature between two pressure levels $\overline{T}_v$ where:

$$\overline{T}_v = \frac{\overline{T}}{1 - 0.01 \cdot RH(1 - 0.622) p_s / \overline{p}}$$ [1]

Here p_s is the saturation pressure for water vapour at $\overline{T}$ calculated according to the formulation of Hyland and Wexler 1983[4]. 0.622 is the ratio of the molar masses of water vapour and dry air, RH is the relative humidity. $\bar{T} = \frac{T_1+T_2}{2}$ and $\bar{p} = \sqrt{p_1 p_2}$. The uncertainty in virtual temperature would have an effect on the final uncertainty in geopotential height but it is assumed small and not accounted for.

Information / data	Type / value / equation	Notes / description
Name of effect	Virtual Temperature	
Contribution identifier	5a, T_v	
Measurement equation parameter(s) subject to effect	Geopotential height	
Contribution subject to effect (final product or sub-tree intermediate product)	Geometric pressure altitude	
Time correlation extent & form	none	
Other (non-time) correlation extent & form	none	
Uncertainty PDF shape	N/A	
Uncertainty & units (1σ)	$u(\bar{T}_v) \approx u(T)$	Based on sensitivity tests using ΔT = u_temp and Δrh = u_rh.
Sensitivity coefficient	1	Uncertainty not included in GRUAN processing
Correlation(s) between affected parameters	Smoothed pressure profile, geopotential height	
Element/step common for all sites/users?	yes	
Traceable to …	Sonde T and RH measurements, p measurements, geopotential height, saturation pressure calculations.	
Validation	N/A	

4.9 Sonde T and RH readings (5a1)

The radiosonde carries a thin film capacitor humidity sensor and a capacitive wire temperature sensor. These are used in calculating mean virtual temperature and the bias of the pressure sensor, but the uncertainties they contribute are assumed small and not accounted for in the final geopotential height uncertainty. The assessment of the uncertainty in the GRUAN temperature or relative humidity product can be found in the relevant PTU documents.

Information / data	Type / value / equation	Notes / description
Name of effect	Sonde T and RH readings	
Contribution identifier	5a1	
Measurement equation	Geopotential height	

parameter(s) subject to effect		
Contribution subject to effect (final product or sub-tree intermediate product)	Virtual temperature	
Time correlation extent & form	none	
Other (non-time) correlation extent & form	none	
Uncertainty PDF shape	normal	
Uncertainty & units (1σ)	Change in ΔH: 0.05 % with change in T, throughout profile. 0.02 % with change in RH, throughout profile. Change in z_p: 5 m at 15 km with change in T. <0.7 m at 15 km with change in RH.	Using sensitivity tests with ΔT=u_cor_temp and ΔRH = u_cor_rh. Correlated uncertainty was used as z is calculated from a sum of many individual steps and it would be expected that the statistical errors in each step cancel out.
Sensitivity coefficient	1	Uncertainty not included in GRUAN processing
Correlation(s) between affected parameters	Also used in bias of the pressure sensor, launch altitude	
Element/step common for all sites/users?	yes	
Traceable to …	GRUAN T and RH measurements.	See temperature and relative humidity traceability documents.
Validation	N/A	

4.10 Local Gravity Calculations (5b)

Local gravity is used in calculating geometric altitude from pressure and the bias of the pressure sensor. It can be found using:

$$\gamma(z_j,\varphi) = 9.780318 \cdot \left(1 + 5.3024 \cdot 10^{-3} sin^2(\varphi) - 5.8 \cdot 10^{-6} sin^2(2\varphi)\right) - 3.085 \cdot 10^{-5} z_j$$ [5]

Where z_{GPS} is used for z_j to avoid recursive calculation.

Information / data	Type / value / equation	Notes / description
Name of effect	Local Gravity Calculations	
Contribution identifier	5b, $\gamma(z_j,\varphi)$	
Measurement equation parameter(s) subject to effect	Geopotential height	

Contribution subject to effect (final product or sub-tree intermediate product)	Geometric pressure altitude	
Time correlation extent & form	none	
Other (non-time) correlation extent & form	none	
Uncertainty PDF shape	N/A	
Uncertainty & units (1σ)	Change in ΔH: $7\text{x}10^{-4}$ % with change in z_{GPS}, throughout profile. $4\text{x}10^{-4}$ % with change in φ, throughout profile. Change in z_p: 0.06 m at 15km with change in z_{GPS} 0.1 m at 15 km with change in φ	Based on sensitivity tests using $\Delta z_{GPS} = 20$ m and $\Delta\varphi = 0.001°$.
Sensitivity coefficient	1	Uncertainty not included in GRUAN processing
Correlation(s) between affected parameters	Smoothed pressure profile	
Element/step common for all sites/users?	yes	
Traceable to …	GPS altitude measurements	
Validation	N/A	

4.11 Launch altitude (5c), $u_u(h_0)$

The launch altitude is calculated from the first sonde pressure reading after launch and the station barometer using the hydrostatic equation and the station barometers altitude. The total uncertainty in launch altitude is determined from the uncertainty of the station barometer, including the uncertainty in the station barometers altitude, and from the random noise of the pressure sensor at launch. ρ_0 is calculated from the sonde pressure and temperature readings at launch and $\gamma(h_{station},\varphi_{station})$ is the local gravity.

Information / data	Type / value / equation	Notes / description
Name of effect	Launch altitude uncertainty	
Contribution identifier	5c, $u_u(h_0)$	
Measurement equation parameter(s) subject to effect	Geopotential height, pressure readings with uncertainties.	
Contribution subject to effect (final product or sub-tree intermediate product)	Geometric pressure altitude	

Time correlation extent & form	Between recalibrations of the station barometer and measurements of the station barometer altitude.	
Other (non-time) correlation extent & form	Throughout sounding	
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	$u_u(h_0) = \sqrt{u_{u,launch}^2\left(z_p\right) + (100 \cdot \frac{u_r(p_1)}{\rho_o \gamma(h_{station}, \emptyset_{station})})^2}$ Typical value < 0.5 m	Geometric sum of uncertainty of station barometer and random noise[1]. $U_u(h_0)$ is included in $u(z_p)$. Assuming p is measured in hectopascals, the factor of 100 scales the measurements to pascals.
Sensitivity coefficient	1	
Correlation(s) between affected parameters	none	
Element/step common for all sites/users?	yes	
Traceable to …	Pre-launch pressure readings, station barometer, local gravity calculations, sonde temperature readings.	
Validation	N/A	

4.12 **GPS altitude at launch (5c1)**

Used in calculating the station local gravity for the uncertainty in launch altitude.

Information / data	**Type / value / equation**	**Notes / description**
Name of effect	GPS altitude at launch	
Contribution identifier	5c1	
Measurement equation parameter(s) subject to effect	Geopotential height	
Contribution subject to effect (final product or sub-tree intermediate product)	Launch altitude	
Time correlation extent & form	none	
Other (non-time) correlation extent & form	none	
Uncertainty PDF shape	normal	

Uncertainty & units (2σ)	20 m[5]	Vertical position uncertainty according to Vaisala RS92 datasheet[6] Used in calculating local gravity, but the uncertainty is not propagated.
Sensitivity coefficient	1	Uncertainty is not used in GRUAN processing.
Correlation(s) between affected parameters	none	
Element/step common for all sites/users?	yes	
Traceable to …	GPS sensor	
Validation	N/A	

4.13 Pre-launch pressure readings (5c2)

The statistical noise is determined from 100 pressure readings taken around the time of launch. Used in determining the uncertainty in the launch altitude.

Information / data	**Type / value / equation**	**Notes / description**
Name of effect	Pre-launch pressure readings	Statistical noise of 100 readings taken around launch time
Contribution identifier	5c2	
Measurement equation parameter(s) subject to effect	Geopotential height	
Contribution subject to effect (final product or sub-tree intermediate product)	Launch height uncertainty	
Time correlation extent & form	none	
Other (non-time) correlation extent & form	none	
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	0.06 hPa	Calculated using typical values of 0.5 m uncertainty, 1.225 kgm^{-3} air density and 9.8 ms^{-2} local gravity.
Sensitivity coefficient	$100/(\rho_0\gamma(h_{station},\varphi_{station}))$	Factor of 100 scales the pressure uncertainty from hectopascals to pascals.
Correlation(s) between affected parameters	none	
Element/step common for all sites/users?	yes	

Traceable to …	Barocap pressure sensor	
Validation	N/A	

4.14 Calculate noise in z_p (6), $u_r(z_p)$

The noise in z_p is calculated using a 100-point wide window so it can be compared to the noise in z_{GPS} to determine the switch altitude. The statistical uncertainty at a point s_i is calculated using[7] (equation A5 in Dirksen et al.):

$$u(\bar{s_i}) = \sqrt{\frac{N'}{N'-1}\sum_{j=-M}^{M} c_j^2 (s_{i+j} - \bar{s_i})^2}$$

Where $N' = (\sum_{j=-M}^{M} c_j^2)^{-1}$ is the effective sample size and c_j normalizes the kernel, so that $\sum c_j = 1$ and $c_{-j} = c_j$.

Information / data	Type / value / equation	Notes / description
Name of effect	Calculate noise in z_p	
Contribution identifier	6, $u_r(z_p)$	
Measurement equation parameter(s) subject to effect	Geopotential height	
Contribution subject to effect (final product or sub-tree intermediate product)	Switch altitude	
Time correlation extent & form	100 measurement points.	
Other (non-time) correlation extent & form	normal	
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	About 0.25 m below z_{switch} but rapidly increases above 15 km altitude to 1.5 m - 2 m	Based on Dirksen et al. 2014 figure 19 – see figure 1.
Sensitivity coefficient	1	
Correlation(s) between affected parameters	none	
Element/step common for all sites/users?	yes	
Traceable to …	Geometric altitude	
Validation	N/A	

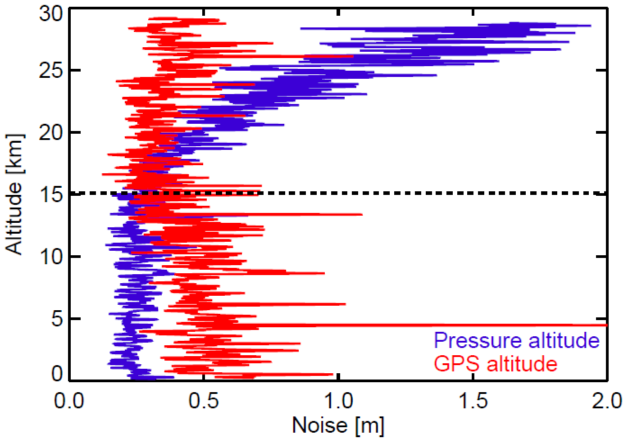


Figure 19. Noise of the geometric altitude derived from the pressure sensor (blue) and the GPS sensor (red). The standard deviation is calculated using Eq. (A5) for a low-pass filter with a cut-off frequency of 0.067 Hz (corresponding to a period of 15 s). The dashed black line indicates the altitude (15.1 km) where the switch from pressure-based to GPS-based altitude occurs. The sounding was performed at Lindenberg on 17 September 2013 at 12:00 UTC.

Figure 4 Dirksen et al. figure 19

4.15 GPS sensor (7)

The RS92-SGP radiosonde uses a code-correlating GPS sensor. Because of accuracy problems in the first few kilometres the geopotential height is only calculated using the GPS measurements for higher altitudes.

Information / data	Type / value / equation	Notes / description
Name of effect	GPS Sensor	
Contribution identifier	7	
Measurement equation parameter(s) subject to effect	Geopotential height	
Contribution subject to effect (final product or sub-tree intermediate product)	Geopotential height	
Time correlation extent & form	none	
Other (non-time) correlation extent & form	none	
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	20 m	Vertical position uncertainty, from Vaisala RS92 data sheet[6].
Sensitivity coefficient	1	Uncertainty is not used in GRUAN processing.

Correlation(s) between affected parameters	Z$_{GPS}$ at launch	
Element/step common for all sites/users?	yes	
Traceable to …	Vaisala	
Validation	N/A	

4.16 GPS altitude measurements (8)

The RS92 GPS takes vertical and horizontal position measurements every second after launch using WGS-84 xyz coordinates. Standard Vaisala processing uses a station GPS antenna as a reference but GRUAN processing uses z_p, calculated from the station barometer, to convert these to altitude. The total uncertainty in the GPS altitude measurements is the geometric sum of the statistical noise of z_{GPS}, the correlated uncertainty at the switch altitude (see section 3.5) and the uncertainty of the offset, which is the statistical uncertainty of z_p-z_{GPS} at the switch altitude.

Information / data	Type / value / equation	Notes / description
Name of effect	GPS measurements	
Contribution identifier	8, z_{GPS}	
Measurement equation parameter(s) subject to effect	Geopotential height,	
Contribution subject to effect (final product or sub-tree intermediate product)	Geometric GPS altitude	
Time correlation extent & form	none	
Other (non-time) correlation extent & form	none	
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	$u(z_{GPS}) = \sqrt{u_r(z_{GPS})^2 + u_c(offset)^2 + u_{c,switch}(z_p)^2}$ Is fairly constant and usually between 10-50 m	This is dominated by the correlated uncertainty[1].
Sensitivity coefficient	1	
Correlation(s) between affected parameters	Local gravity calculations	
Element/step common for all sites/users?	yes	
Traceable to …	GPS sensor, switch altitude, offset calculation	
Validation	Altitude from pressure.	

4.17 Calculate Noise in Z_{GPS} (9), $u_r(Z_{GPS})$

The statistical noise in z_{GPS} calculated over a 100 point window using the same method described in section 4.12

Information / data	Type / value / equation	Notes / description
Name of effect	Calculate noise in z_{GPS}	
Contribution identifier	9, $u_r(z_{GPS})$	
Measurement equation parameter(s) subject to effect	Geopotential height	
Contribution subject to effect (final product or sub-tree intermediate product)	Switch altitude	
Time correlation extent & form	none	
Other (non-time) correlation extent & form	100 measurement points.	
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	0.4 m	Based on Dirksen et al. 2014 figure 19, see Figure 1.
Sensitivity coefficient	1	
Correlation(s) between affected parameters	none	
Element/step common for all sites/users?	none	
Traceable to …	z_{GPS}	
Validation	N/A	

4.18 Switch altitude (10), z_{switch}

The switch altitude is the altitude at which geometric pressure altitude stops being used and geometric GPS altitude starts being used instead. This is determined as the first level above 3km where the statistical noise in z_{GPS} exceeds the statistical noise in z_p by less than 20%. Usually lies between 9km and 17km. See Figure 1 for example.

Information / data	Type / value / equation	Notes / description
Name of effect	Switch altitude	
Contribution identifier	10, z_{switch}	
Measurement equation parameter(s) subject to effect	Geopotential height, pressure readings with uncertainties	
Contribution subject to effect (final product or sub-tree intermediate product)	Geometric GPS altitude	

Time correlation extent & form	none	
Other (non-time) correlation extent & form	Sounding above switch altitude	
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	$U_{c,switch}(z_p)$, <10-50 m	The correlated uncertainty of the geometric pressure altitude at the switch altitude. Is included in $u(z_{GPS})$ so has to be smaller[1].
Sensitivity coefficient	1	
Correlation(s) between affected parameters	none	
Element/step common for all sites/users?	yes	
Traceable to …	Z_p, z_{GPS}	Depends on the noise in z_p and in z_{GPS}.
Validation	N/A	

4.19 Geometric altitude offset (11), z_{offset}

The offset is the difference between the geometric pressure altitude and the GPS altitude measurement at the switch altitude. Typically has a value of about 50m. The uncertainty of the offset is the statistical uncertainty of z_p-z_{GPS} at the switch altitude, z_{switch}.

Information / data	Type / value / equation	Notes / description
Name of effect	Geometric altitude offset	
Contribution identifier	11, z_{offset}	
Measurement equation parameter(s) subject to effect	Geopotential height, pressure readings with uncertainties.	
Contribution subject to effect (final product or sub-tree intermediate product)	Geometric GPS altitude.	
Time correlation extent & form	None.	
Other (non-time) correlation extent & form	Sounding above switch altitude.	
Uncertainty PDF shape	Normal.	
Uncertainty & units (1σ)	< 10-50 m	Since u_c(offset) is included in $u(z_{GPS})$ the value has to be smaller than the total uncertainty.
Sensitivity coefficient	1	
Correlation(s) between affected	none	

parameters		
Element/step common for all sites/users?	yes	
Traceable to …	Z_p, z_{GPS},	
Validation	N/A	

4.20 Join Pressure and GPS profiles at the switch altitude (12), z

Joining pressure and GPS altitude profiles produces the geophysical altitude. The geophysical altitude is then z_p below the switch altitude and $z_{GPS}+z_{offset}$ above.

Information / data	Type / value / equation	Notes / description
Name of effect	Join z_p and z_{GPS} at the switch altitude	
Contribution identifier	12, z	
Measurement equation parameter(s) subject to effect	Geopotential height	
Contribution subject to effect (final product or sub-tree intermediate product)	Geopotential height	
Time correlation extent & form	none	
Other (non-time) correlation extent & form	none	
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	$U(z_p)$ below z_{switch} $U(z_{GPS})$ above z_{switch} 10-50 m (<35 usually)	For example values see Figure 2. 10-50 m range based on Dirksen et al. Data files show u_alt usually below 35 m. Both are dominated by correlated uncertainty.
Sensitivity coefficient	1	
Correlation(s) between affected parameters	none	
Element/step common for all sites/users?	yes	
Traceable to …	$Z_p, z_{GPS}, z_{switch}, z_{offset}$	
Validation	N/A	

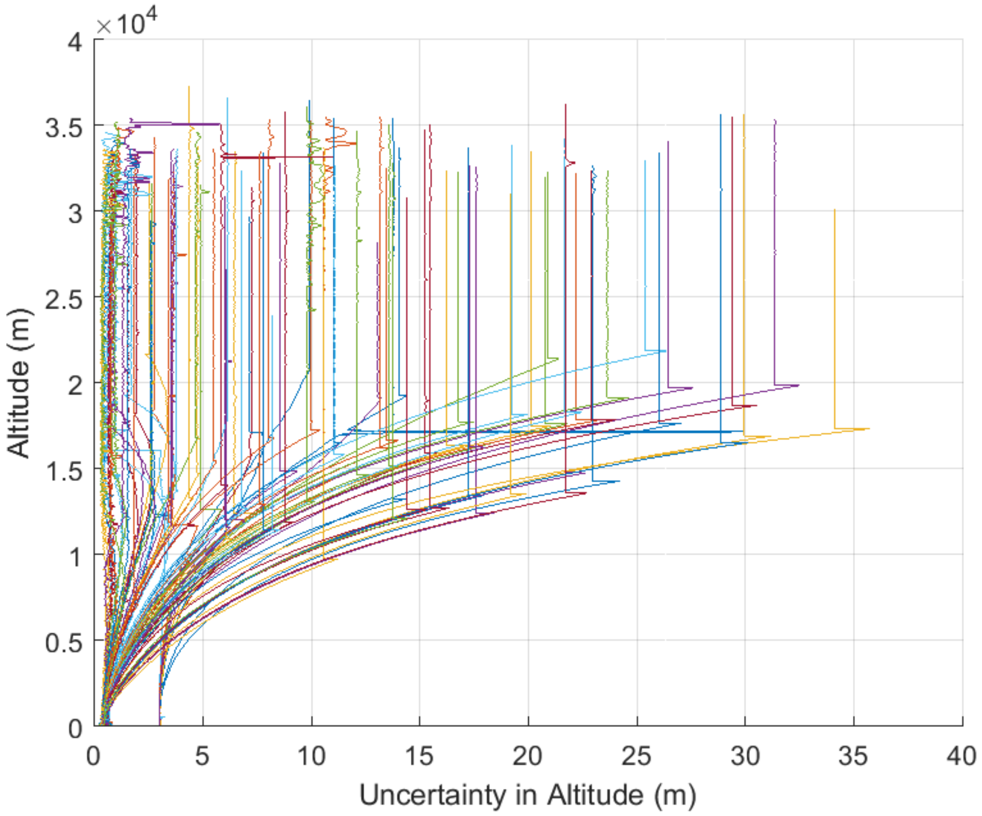


Figure 5. typical examples of uncertainty in altitude, u_alt, with altitude, taken from a sample of RS92 radiosondes launched at Lindenberg between 2012 and 2017.

4.21 Smoothed pressure profile (13), p

Geometric altitude is converted into a smoothed pressure profile before being converted into geopotential height. The pressure difference between two altitude levels is calculated using:

$$\Delta p_{j-1,j} = p_j[\exp\left(\frac{\gamma\left(z_j,\varphi\right)\cdot\Delta z_{j,j-1}}{R_d\cdot\bar{T}_{v,j}}\right)-1]$$

The uncertainty in p is then determined using u(z), where z is z_p below the switch altitude and z_{GPS} above it.

Information / data	Type / value / equation	Notes / description
Name of effect	Conversion to smoothed pressure profile	
Contribution identifier	13, p	
Measurement equation parameter(s) subject to effect	Geopotential height	
Contribution subject to effect (final product or sub-tree intermediate product)	Geopotential height	

Time correlation extent & form	none	
Other (non-time) correlation extent & form	Degree of smoothing	
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	$u(p) = \sqrt{(u_{c,GC25}(p))^2 + (\frac{\gamma_{45} \cdot p}{R_d \cdot T} \cdot \exp\left(-\frac{\gamma_{45} \cdot dz}{R_d \cdot T}\right) \cdot u(z))^2}$ < 0.6 hPa	For values see figure 3.
Sensitivity coefficient	1	
Correlation(s) between affected parameters	none	
Element/step common for all sites/users?	Yes	
Traceable to …	Geophysical altitude, GC25 calibration	
Validation	N/A	

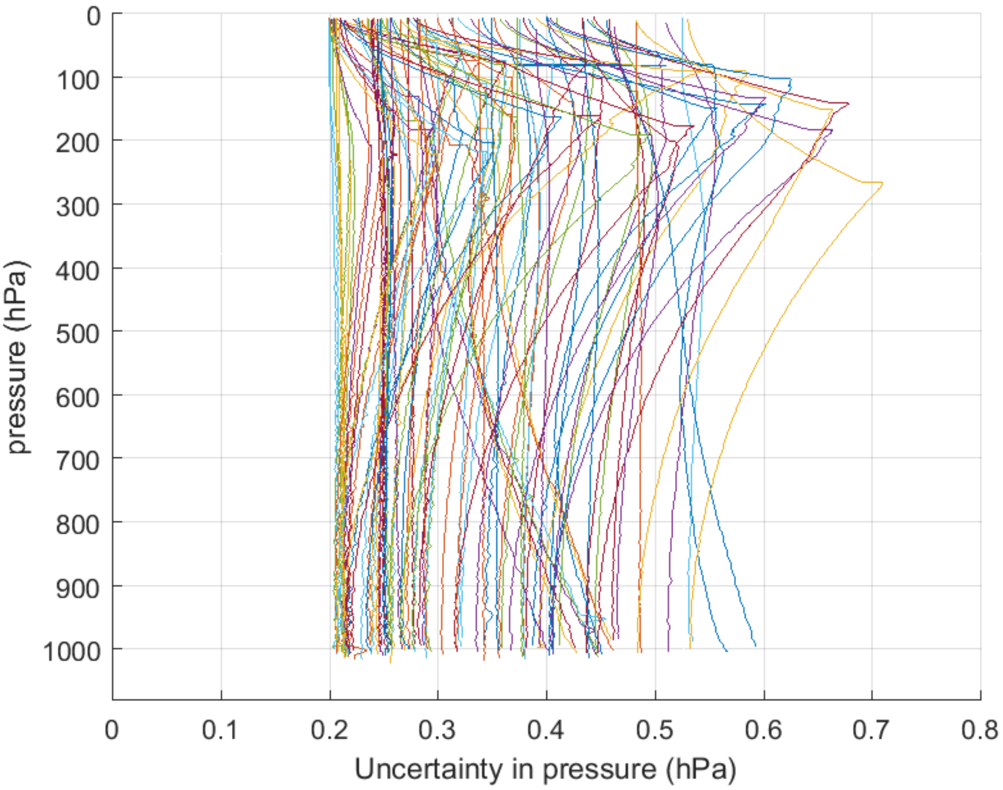


Figure 6, typical examples of uncertainty in pressure, u_press, taken from a sample of RS92 radiosondes launched at Lindenberg between 2012 and 2017.

4.22 Geopotential height (14) H

The geopotential height is calculated from the smoothed pressure profile using:

$$\Delta H_{1,2} = \frac{R_d}{\gamma_{45}} \overline{T_v} ln(\frac{p_1}{p_2})$$ [8]

Where R_d is the gas constant of dry air, γ_{45} the normal gravity at 45.542° latitude, and $\overline{T_v}$the average virtual temperature between the levels p_1 and p_2.

Information / data	Type / value / equation	Notes / description
Name of effect	Geopotential height	
Contribution identifier	14, H	
Measurement equation parameter(s) subject to effect	none	End product
Contribution subject to effect (final product or sub-tree intermediate product)	none	
Time correlation extent & form	none	
Other (non-time) correlation extent & form	Degree of smoothing	
Uncertainty PDF shape	normal	
Uncertainty & units (2σ)	$u(z_p)$ for $z < z_{switch}$ $u(z_{GPS})$ for $z > z_{switch}$ 10-50 m (<35 usually)	The uncertainty in geopotential height is stated to be identical to the uncertainty in geometric altitude
Sensitivity coefficient	1	
Correlation(s) between affected parameters	none	
Element/step common for all sites/users?	yes	
Traceable to …	Geometric altitude from pressure and GPS measurements.	
Validation	N/A	

5 Uncertainty summary

Element Identifier	Contribution name	Uncertainty contribution form	Typical value	Traceability level (L/M/H)	Random, structured random, quasi-systematic or systematic?	Correlated to?
1	Barocap pressure sensor, u_{cal}	Statistical uncertainty	0.5 hPa > 100 hPa, 0.3 < 100 hPa	H	random	none
2	Calibrated in Vaisal CAL4 facility	constant	0.4 hPa > 100 hPa, 0.3 < 100 hPa	H	Systematic	4
2a	Reference pressure sensors	constant	0.3 hPa	H	systematic	2,4
3	GC25 Calibration, $U_{c,GC25}(p)$	$\sqrt{u_{cal}^2 + (\frac{\Delta p_{GC25}}{3})^2}$	0.43 hPa	H	Quasi-systematic	12
3a	Station barometer, $u_{u,launch}(z_p)$	constant	<0.5 m	H	systematic	5c
4	Pressure measurements	Statistical uncertainty	1 hPa > 100 hPa, 0.6 < 100 hPa	H	random	5a
5	Calculate geometric altitude, $u(z_p)$	$\sqrt{u_u(h_0)^2 + u_r(z_p)^2 + u_c(z_p)^2}$	0.5 at launch up to $u(z_{GPS})$ at z_{switch}.	M	Structured-random	9,10,11
5a	Virtual Temperature	constant	0 m	L	random	12,13
5a1	Sonde T and RH readings	constant	0 m	L	random	5c
5b	Local Gravity Calculations	constant	0 m	L	random	12
5c	Launch altitude, $u_u(h_0)$	$\sqrt{u_{u,launch}^2(z_p) + (100 \cdot \frac{u_r(p_1)}{\rho_o \gamma(h_{station}, \emptyset_{station})})^2}$	<0.5 m	M	Structured-random	none
5c1	GPS altitude at launch	constant	0 m	L	random	none
5c2	Pre-launch pressure readings	Statistical uncertainty	0.5 hPa	H	random	none
6	Calculate noise in z_p	Statistical uncertainty	0.25 m	M	random	none
7	GPS sensor	constant	20 m	H	random	5c1
8	GPS altitude measurements, $u(z_{GPS})$	$\sqrt{u_r(z_{GPS})^2 + u_c(offset)^2 + u_{c,switch}(z_p)^2}$	10-50 m	M	Structured random	5b
9	Calculate noise in z_{GPS}	Statistical uncertainty	0.5 m	M	random	none
10	Switch altitude, $u_{c,switch}(z_p)$	Correlated uncertainty in z_p at z_{switch}	<10-50 m	M	Quasi-systematic	none
11	Geometric altitude offset, $u_c(offset)$	Statistical uncertainty of z_p-z_{GPS} at z_{switch}	<10-50 m	M	Quasi-systematic	none
12	Join z_p and z_{GPS} at the switch altitude, $u(z)$	$U(z_p)$ below switch altitude $U(z_{GPS})$ above switch altitude	10-50 m	M	Structured random	none

13	Smoothed pressure profile, u(p)	$\sqrt{(u_{c,GC25}(p))^2 + (\frac{\gamma_{45} \cdot p}{R_d \cdot T} \cdot \exp\left(-\frac{\gamma_{45} \cdot dz}{R_d \cdot T}\right) \cdot u(z))^2}$	0.6 hPa	M	Structured random	none
14	Geopotential height	U(z_p) below switch altitude U(z_{GPS}) above switch altitude	10-50 m	M	Structured random	none

How the uncertainty in Geopotential height and altitude is calculated depends on whether it is above or below the switch altitude, z_{switch}. Below z_{switch} the uncertainty is the sum in quadrature of the uncertainty in launch height altitude and from the bias of the pressure sensor, as well as the noise in pressure measurements. Above z_{switch} the uncertainty is the sum in quadrature of the uncertainties in the switch altitude and the offset between altitude from pressure measurements and altitude from GPS, with random noise in GPS altitude measurements.

$$U(H) = \begin{cases} \sqrt{u_u(h_0)^2 + u_r(z_p)^2 + u_c(z_p)^2}, z < z_{switch} \\ \sqrt{u_r(z_{GPS})^2 + u_c(offset)^2 + u_{c,switch}(z_p)^2}, z > z_{switch} \end{cases}$$

The uncertainty in pressure is the sum in quadrature of the uncertainty from the calibration during ground check and an uncertainty contribution determined from the uncertainty in altitude as shown below.

$$U(p) = \sqrt{(u_{c,GC25}(p))^2 + (\frac{\gamma_{45} \cdot p}{R_d \cdot T} \cdot \exp\left(-\frac{\gamma_{45} \cdot dz}{R_d \cdot T}\right) \cdot u(z))^2}$$

The uncertainty in geometric altitude usually starts at launch around 0.5 m and increases with altitude up to the switch altitude, usually between 10 and 50 m. Most of this uncertainty is the correlated uncertainty resulting from the bias of the pressure sensor. Together random noise and launch height uncertainty contribute less than 20% of the total uncertainty. Above the switch altitude the uncertainty remains fairly constant, with some change as a result of random noise so the uncertainty here is between 10 and 50 m. Less than 5% of this is the uncertainty due to random noise while the rest is correlated uncertainty from the bias of the pressure sensor at the switch altitude and the uncertainty in the offset. The uncertainty in geopotential height is the same as in geometric altitude, starting at about 0.5 m rising up to between 10 to 50 m and then staying fairly constant. The uncertainty in pressure depends on the uncertainty in altitude and increases up to the switch altitude. Above the switch altitude the uncertainty in pressure decreases. The maximum uncertainty in pressure is usually below 0.6 hPa. Depending on altitude between 30% and 90% of the uncertainty is correlated uncertainty from the ground check and long term systematic uncertainty from the Vaisala calibration. The remaining uncertainty is broken down into correlated and uncorrelated uncertainty the same as u(z_p) below z_{switch} and u(z_{GPS}) above z_{switch}.

6 Traceability uncertainty analysis

Traceability level definition is given in Table 2.

Table 2. Traceability level definition table

Traceability Level	Descriptor	Multiplier
High	SI traceable or globally recognised community standard	1

Medium	Developmental community standard or peer-reviewed uncertainty assessment	3
Low	Approximate estimation	10

Analysis of the summary table would suggest the following contributions, shown in table 2, should be considered further to improve the overall uncertainty of the GRUAN temperature product. The entries are given in an estimated priority order.

Table 3 Traceability level definition further action table.

Element identifier	Contribution name	Uncertainty contribution form	Typical value	Traceability level (L/M/H)	Random, structured random, quasi-systematic or systematic?	Correlated to?
3	GC25 Calibration, $U_{c,GC25}(p)$	$\sqrt{u_{cal}^2 + (\frac{\Delta p_{GC25}}{3})^2}$	0.43 hPa	H	Quasi-systematic	12
7	GPS sensor	constant	20 m	H	random	5c1
5c1	GPS altitude at launch	constant	0 m	L	random	none
5a	Virtual Temperature	constant	0 m	L	random	12,13
5b	Local Gravity Calculations	constant	0 m	L	random	12

6.1 Recommendations

Calculating altitude from pressure uses virtual temperature which is calculated from temperature and relative humidity measurements, however no attempt is made to incorporate the uncertainty of these inputs into the uncertainty of the end product, and although sensitivity tests indicate that both would only have a small change on each calculated ΔZ, the number of steps means the uncertainty in z_p could be significant near the switch altitude.

There are also points in Dirksen et al. where the methods used are not fully clear or justified, particularly relating to the correlated uncertainty of the pressure sensor, where it is not obvious how the difference in ground check readings can be used as a contributor to uncertainty in the way it has been, and how the bias of the pressure sensor is interpolated linearly to it when it is apparently based on calculations of z_p-z_{GPS} throughout the entire profile.

The application of z_{offset} to all readings above the switch altitude introduces a correlated uncertainty to all high altitude readings. An alternative method that combines z_p and z_{GPS} in the switch region, with z_p used below and z_{GPS} used above, would goive improved uncertainties at higher altitudes.

It would also be useful if some of the data used to calculate the different uncertainties, such as at the ground check and switch altitude, were made available.

There are 4 contributions that do not have an assigned uncertainty. Some analysis to determine the magnitude of these potential contributions would better constrain the uncertainty budget.

Some contributions are discussed, but not used in the overall uncertainty calculation, e.g. uncertainty from the temperature product. The uncertainty contribution from these elements should be quantified and used.

7 Conclusion

The GRUAN RS92 radiosonde geopotential height product has been assessed against the GAIA CLIM traceability and uncertainty criteria.

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Product Traceability and Uncertainty for the Microwave Radiometer (MWR) brightness temperature product

Version 1.0

GAIA-CLIM
Gap Analysis for Integrated
Atmospheric ECV Climate Monitoring
Mar 2015 - Feb 2018

A Horizon 2020 project; Grant agreement: 640276

Date: 30 November 2017

Dissemination level: PU

Work Package 2; Task 2.1.2; Complied by Domenico Cimini (CNR)

Consiglio Nazionale delle Ricerche

Table of Contents

Version history

Version	Principal updates	Owner	Date
0.1 draft	First draft	CNR	28.03.2017
0.2 draft	Second draft	CNR	31.03.2017
0.3 draft	Third draft - sent for initial external comments	CNR	16.06.2017
0.4 draft	Forth draft – adapted to format provided by NPL	CNR	28.06.2017
0.5 draft	Fifth draft – after comments from Paul Green (NPL)	CNR	27.07.2017
0.6 draft	Sixth draft – after Webex meeting on Oct 9th 2017	CNR	31.10.2017
1.0	First issue as annex E of D2.6	CNR	30.11.2017

1 Product overview

Product name: MWR brightness temperature product
Product technique: Measurement of downwelling brightess temperature at multiple frequency channels
Product measurand: Brightess temperature
Product form/range: Multiple channels in the 20-60 GHz spectrum
Product dataset: TOPROF data set
Site/Sites/Network location:

SITE	LAT	LON	HEIGHT(m)	MWR	LOCATION	COUNTRY
JOYCE	50.91	6.41	111	HATPRO G2	Juelich	DE
LACROS	51.35	12.43	125	HATPRO G2	Liepzig	DE
Payerne	46.82	6.95	491	HATPRO G1	Payerne	CH
SIRTA	48.80	2.36	156	HATPRO G2	Paris	FR
CESAR	51.97	4.93	-0.7	HATPRO G1	Cabauw	NL
RAO	52.21	14.12	125	MP3000A	Lindenberg	DE

Product time period: Jan 1, 2015 – Feb 27, 2016
Data provider: TOPROF
Instrument provider: Site management
Product assessor: Domenico Cimini, CNR
Assessor contact email: domenico.cimini@imaa.cnr.it

1.1 Guidance notes

For general guidance see the Guide to Uncertainty in Measurement & its Nomenclature, published as part of the GAIA-CLIM project.

This document is a measurement product technical document which should be stand-alone i.e. intelligible in isolation. Reference to external sources (preferably peer-reviewed) and documentation from previous studies is clearly expected and welcomed, but with sufficient explanatory content in the GAIA CLIM document not to necessitate the reading of all these reference documents to gain a clear understanding of the GAIA CLIM product and associated uncertainties entered into the Virtual Observatory (VO).

In developing this guidance, we adopted the convention proposed by the QA4ECV project (http://www.qa4ecv.eu/) through the Traceability and Uncertainty Propagation Tool (TUPT). This convention is summarized in Figure 1.

QA4ECV TUPT convention

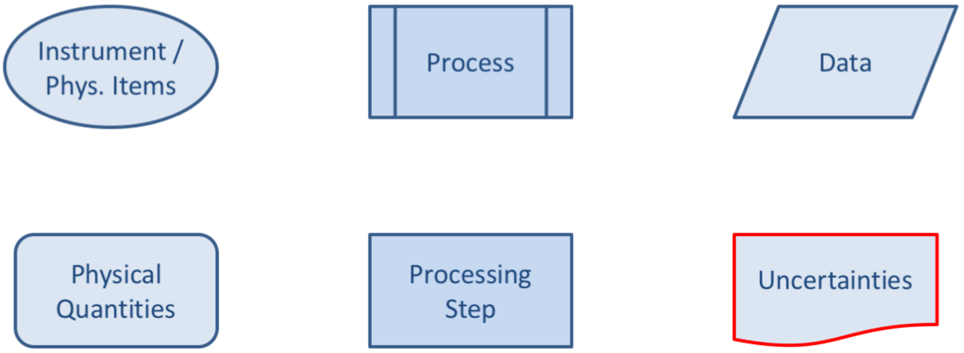

Figure 1. The convention proposed by the QA4ECV project (http://www.qa4ecv.eu/) through the Traceability and Uncertainty Propagation Tool (TUPT). This convention is adopted hereafter to draw the MWR model diagram.

The contribution table to be filled for each traceability contributor has the form seen in Table 1.

Table 1. The contributor table.

Information / data	Type / value / equation	Notes / description
Name of effect		
Contribution identifier		
Measurement equation parameter(s) subject to effect		
Contribution subject to effect (final product or sub-tree intermediate product)		
Time correlation extent & form		
Other (non-time) correlation extent & form		
Uncertainty PDF shape		
Uncertainty & units		
Sensitivity coefficient		
Correlation(s) between affected parameters		
Element/step common for all sites/users?		
Traceable to …		
Validation		

Name of effect – The name of the contribution. Should be clear, unique and match the description in the traceability diagram.

Contribution identifier - Unique identifier to allow reference in the traceability chains.

Measurement equation parameter(s) subject to effect – The part of the measurement equation influenced by this contribution. Ideally, the equation into which the element contributes.

Contribution subject to effect – The top level measurement contribution affected by this contribution. This can be the main product (if on the main chain), or potentially the root of a side branch contribution. It will depend on how the chain has been sub-divided.

Time correlation extent & form – The form & extent of any correlation this contribution has in time.

Other (non-time) correlation extent & form – The form & extent of any correlation this contribution has in a non-time domain. For example, spatial or spectral.

Uncertainty PDF shape – The probability distribution shape of the contribution, Gaussian/Normal Rectangular, U-shaped, log-normal or other. If the form is not known, a written description is sufficient.

Uncertainty & units – The uncertainty value, including units and confidence interval. This can be a simple equation, but should contain typical values.

Sensitivity coefficient – Coefficient multiplied by the uncertainty when applied to the measurement equation.

Correlation(s) between affected parameters – Any correlation between the parameters affected by this specific contribution. If this element links to the main chain by multiple paths within the traceability chain, it should be described here. For instance, SZA or surface pressure may be used separately in a number of models & correction terms that are applied to the product at different points in the processing.

Element/step common for all sites/users – Is there any site-to-site/user-to-user variation in the application of this contribution?

Traceable to – Describe any traceability back towards a primary/community reference.

Validation – Any validation activities that have been performed for this element?

2 Introduction

This document presents the Product Traceabililty and Uncertainty (PTU) information for the Microwave Radiometer (MWR) brightness temperature product. The aim of this document is to provide supporting information for the users of this product within the GAIA-CLIM VO.

Using the convention in Figure 1, the main chain of the MWR instrument is pictured in Figure 2. The red boxes indicate the two main processes:

A) Calibration: the conversion from raw voltages corresponding to the received atmospheric radiance into calibrated brightness temperature (T_B);
B) Inversion: the inversion of calibrated T_B with the combination of some a priori knowledge to estimate the atmospheric products (retrievals).

Thus, MWR uncertainties are here divided in two groups: those affecting the MWR calibration (i.e. from atmospheric radiance to calibrated T_B) and those affecting the retrieval method (from calibrated T_B to MWR retrievals).
As T_B is the primary product of MWR instruments, the process A is treated in this document, while the process B is treated in three child documents (one for each product).

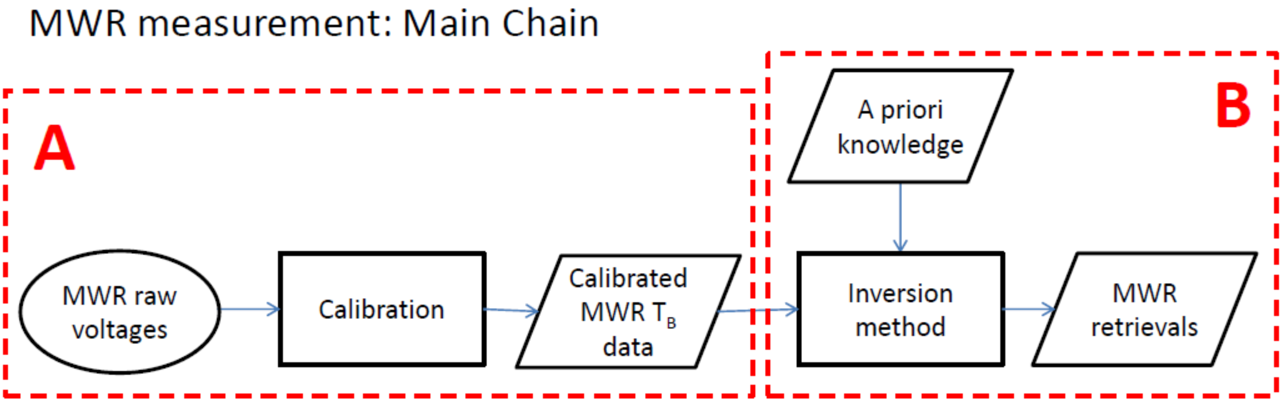

Figure 2. The main chain of the MWR instrument model diagram. The main chain displays the process of producing a geophysical product from the MWR instrument measurements. The process A (from raw voltages to calibrated brightness temperature Tb) is treated in this document. The process B is treated in children documents.

3 Instrument description

Ground-based microwave radiometers (MWR) are instruments calibrated to measure the natural down-welling thermal emission from the atmosphere. The quantity measured by a MWR is atmospheric radiance [W/(m^2·sr·Hz)], which is typically converted into brightness temperature (T_B, [K]) to adopt more familiar units.
Atmospheric temperature and humidity profiles, as well as column-integrated Total Water Vapour Content (TWVC) and Total Liquid Water Content (TLWC), can be inferred from ground-based MWR T_B observations.
Review articles on MWR measurements are given by Westwater et al., 2004 & 2005. Common MWR commercial units operate several channels in the 20-60 GHz frequency range. The 20-30 GHz range is sometimes referred to as K-band, while the 50-60 GHz range is called V-band.

A typical MWR calibration equation is given by:

$$T_B = \left(\frac{U_S}{g}\right)^{\frac{1}{\alpha}} - T_R$$

where:
T_B is the calibrated brightness temperature;
α is the detector non-linearity parameter;
U_S is the measured scene voltage;
g is the gain;
T_R is the system noise temperature.
The calibration parameters g, α, and T_R are determined through the MWR calibration.
MWRs are generally calibrated by so-called hot-cold calibration. Ideally, assuming the detector behaves linearly (α=1), two reference points spanning the full atmospheric measurement range are

sufficient. The hot-cold method exploits two targets, one at hot or ambient temperature (T_H) and the other at cold cryogenic temperature (T_C), usually obtained by a liquid nitrogen (LN2) bath. To consider the detector non-linearity additional calibration points are needed, which are obtained by adding noise from a noise diode source while observing the two calibration targets. This method provides four reference points (4-point calibration) that are needed to solve for the four parameters g, α, and T_R and the noise diode equivalent temperature (T_N). Another calibration method, the so-called tipping curve calibration, exploits the relationship between atmospheric opacity and elevation angle at relatively transparent frequencies to refine one calibration factor. Details on these calibration methods may be found in Han and Westwater (2000), Hewison and Gaffard (2003), Maschwitz et al. (2013), and Küchler et al. (2015). For estimating the uncertainties affecting the MWR calibration, the uncertainties of the calibration parameters are propagated through these two common calibration procedures, i.e. the hot-cold and the tipping curve methods.

Figure 3 provides details of the MWR measurement metrological model chain for the calibration process (A). It describes the flow diagram of the T_B measurement, including uncertainty sources (highlighted in red) and linkages to reference standards (dashed lines, meanining the traceability to SI is not established yet).

4 Product Traceability Chain

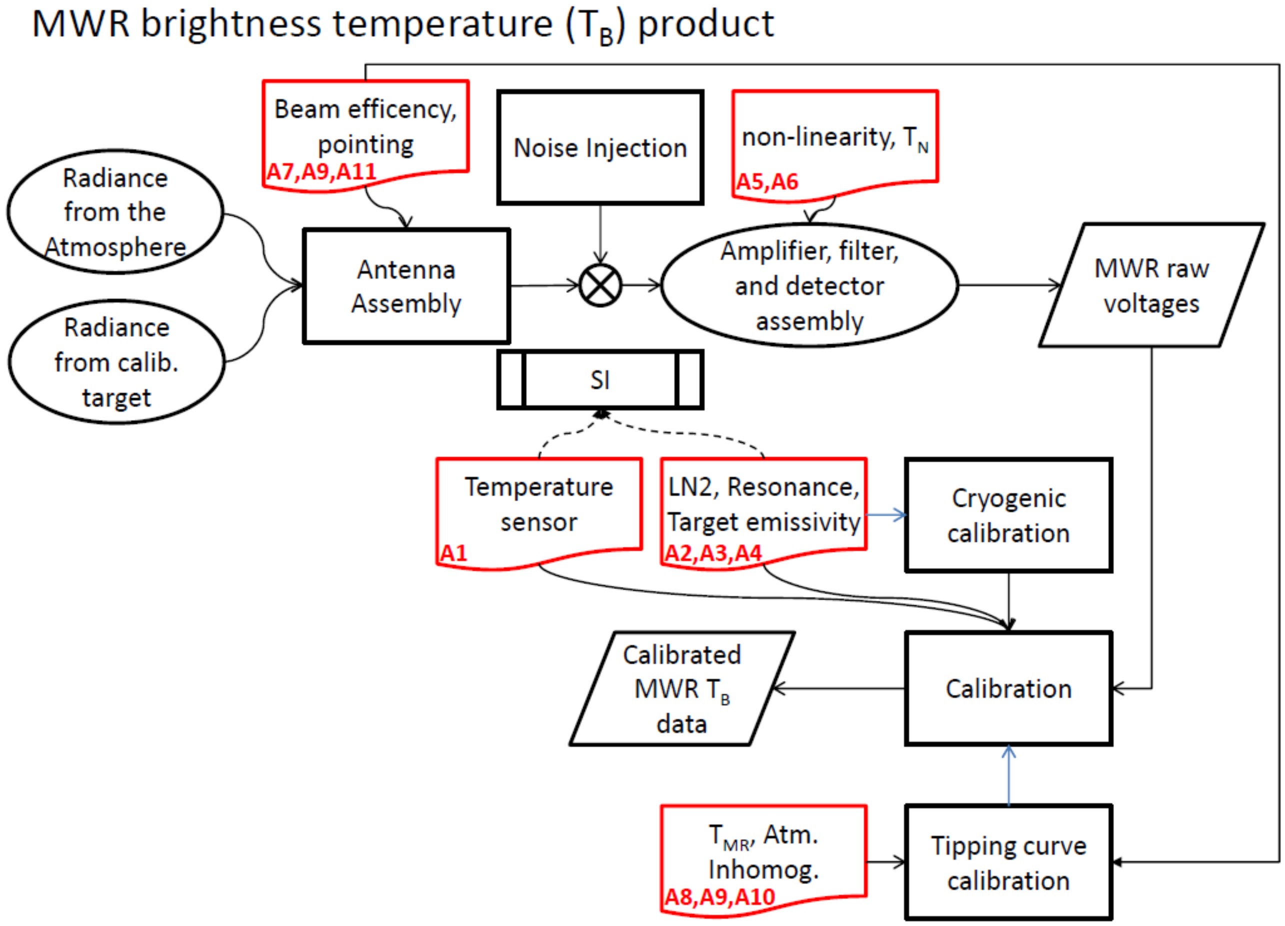

Figure 3. The metrological model chain of the MWR measurement. It describes the flow diagram of the measurement, including uncertainty sources and linkages to reference standards. The dashed lines indicate that the traceability to SI is not established yet.

5 Element contributions

5.1 Temperature sensor (A1)

Calibration uses an internal target at ambient temperature as a hot reference. The main source of uncertainty is the in-situ temperature measurement of the target. An uncertainty of ±0.2 K is considered for the in-situ temperature measurement, which corresponds to the maximum difference typically found between two temperature sensors within the ambient target. The resulting T_B uncertainty is approximately ±0.2K for V-band opaque channels. All other channels are affected by approximately ±0.1 K (Maschwitz et al., 2013). Certified temperature sensors must be deployed to establish traceability to SI. To our our knowledge, certified temperature sensors are not currently deployed on commercial MWR.

Information / data	Type / value / equation	Notes / description
Name of effect	Temperature sensor	
Contribution identifier	A1	
Measurement equation parameter(s) subject to effect	T_H	
Contribution subject to effect (final product or sub-tree intermediate product)	Calibrated T_B	
Time correlation extent & form	None	Random
Other (non-time) correlation extent & form	None	Random
Uncertainty PDF shape	Normal	
Uncertainty & units	±0.1 K (1σ) – K-band ±0.1-0.2 K (1σ) – V-band	Maschwitz et al., 2013
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	Reference temperature sensor	Calibration in manufacturer's facility
Validation	Sensitivity study	Maschwitz et al., 2013

5.2 Target emissivity (A2)

Calibration targets are assumed to be ideal black bodies, while their emissivity ε and reflectivity *r* slightly differ respectively from 1 and 0. Manufacturers specifications give target reflectivity levels lower than -40 dB for frequencies higher than 8 GHz (i.e. $r<0.0001$ and $\varepsilon>0.9999$). The effective T_B is within 0.01 K if the ambient temperature varies from -30 to 40 °C. Therefore, the impact is assumed negligible. However, specifications in the spectral range of the observed MWR channels are not available to our knowledge.

Information / data	Type / value / equation	Notes / description
Name of effect	Non-ideal target emissivity	
Contribution identifier	A2	
Measurement equation parameter(s) subject to effect	T_C, T_H	$T_{Heff} = \varepsilon T_H + (1-\varepsilon)T_{Bamb}$ $T_{Ceff} = \varepsilon T_C + (1-\varepsilon)T_{Bamb}$
Contribution subject to effect (final product or sub-tree intermediate product)	Calibrated T_B	
Time correlation extent & form	None	Systematic
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Rectangular	Assumed
Uncertainty & units (1σ)	±0.02 K (1σ)	
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	Manufacturer specifications	NIST is working on MW standards that shall be able to serve as primary and secondary standards
Validation	None	NIST secondary standards may be used in the future

5.3 LN2 refractive index (A3)

The refractive index of liquid nitrogen (n_{LN2}) determines the reflectivity of the cold target's surface. The value for $n_{LN2} = 1.2$ is derived from laboratory measurements with an uncertainty of ±0.03 (Benson et al., 1983). The resulting T_B uncertainty is 0.7K at K-band channels, and it decreases linearly with higher T_B values. For the opaque channels in the V-band the uncertainty reduces to 0.1 K, and it disappears at the hot calibration point (Maschwitz et al., 2013).

Information / data	Type / value / equation	Notes / description
Name of effect	LN2 refractive index	
Contribution identifier	A3	
Measurement equation parameter(s) subject to effect	$r_{LN_2}=(n_{LN_2}-1)^2/(n_{LN_2}+1)^2$ $T_C=(1-r_{LN_2})T_{LN_2}+r_{LN_2}T_{rec}$	Maschwitz, 2012
Contribution subject to effect (final product or sub-tree intermediate product)	Calibrated T_B	
Time correlation extent & form	None	Systematic
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	Benson et al., 1983
Uncertainty & units (1σ)	±0.7 K (1σ) – K-band ±0.1-0.6 K (1σ) – V-band	Maschwitz et al., 2013
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	Laboratory measurements	Benson et al., 1983
Validation	Intercomparison study	Maschwitz, 2012

5.4 Resonance (A4)

During the cryogenic calibration, LN2 evaporates and its level diminishes, changing its distance to the receiver and the resonance conditions. This affects the uncertainty of the calibration point. The maximum uncertainty is estimated to be twice the amplitude of the oscillation observed at each channel, because the integration time within the LN2 calibration is small compared to the oscillation periods (~2-6 min depending on wavelength; Pospichal et al., 2012). K-band channels show oscillation amplitudes of 0.1 to 0.6 K. In the V-band the amplitudes are 0.1 to 0.3 K (Maschwitz et al., 2013). This effect is suppressed in new generation cryogenic targets, thanks to the employment of polarised anti-reflection coating, though these targets only became commercially available since 2016.

Information / data	Type / value / equation	Notes / description
Name of effect	Resonance	
Contribution identifier	A4	
Measurement equation parameter(s) subject to effect	T_C	
Contribution subject to effect (final product or sub-tree intermediate product)	Calibrated T_B	
Time correlation extent & form	Sinusoidal	Pospichal et al., 2012 Küchler et al., 2015 Paine et al., 2014
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	U-shaped	
Uncertainty & units (1σ)	±0.1-0.8 K (1σ) – K-band ±0.1-0.3 K (1σ) – V-band	Maschwitz et al., 2013
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	N/A	
Validation	Laboratory experiments	Pospichal et al., 2012 Küchler et al., 2015 Paine et al., 2014

5.5 Detector non-linearity (A5)

The relationship between input power (radiance) and detector output voltage slightly deviates from the ideal linear relationship. If the non-linearity is not accounted for in the calibration equation (e.g. through the two-point calibration) this effect leads to substantial systematic uncertainty, of the order of 0.5-0.6 K in the K-band, 0.01-0.40 K in the V-band (Hewison and Gaffard, 2003). However, the detector non-linearity impact can be accounted for through the non-linearity parameter α, whose value is estimated through the four-point calibration. The uncertainty in determining α is 0.1–0.2 % of the mean α value of each frequency channel. At K-band channels the effect ranges between ±0.02 K and ±0.04 K. In the V-band, the effect is below ±0.02 K. Thus, in general the effect of uncertainties on detector non-linearity does not exceed ±0.04 K and it is therefore deemed as negligible (Maschwitz et al. 2013).

Information / data	Type / value / equation	Notes / description
Name of effect	Detector non-linearity	
Contribution identifier	A5	
Measurement equation parameter(s) subject to effect	A	
Contribution subject to effect (final product or sub-tree intermediate product)	Calibrated T_B	
Time correlation extent & form	None	Quasi-systematic
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	±0.04 K (1σ)	Maschwitz et al., 2013
Sensitivity coefficient	1	
Correlation(s) between affected parameters	A6	Detector non-linearity and noise diode temperature are determined through calibration at the same time
Element/step common for all sites/users?	Yes	
Traceable to …	None	
Validation	Sensitivity study	Maschwitz et al., 2013

5.6 Noise diode temperature (A6)

The noise diode temperature T_N is calibrated through the LN2 calibration. The impact of T_N uncertainty is estimated to be negligible for opaque channels, whose calibration is dominated by the ambient target temperature, and ranging between 0.2 and 0.4 K for the non-opaque channels. After the initial LN2 calibration, the measurement accuracy depends on the stability of the injected noise, which is characterized by T_N.

As the LN2 calibration is impractical to perform frequently, the stability is rather important for V-band channels which cannot be calibrated by the tipping curve calibration. A trend analysis of T_N showed +0.006 to +0.010 K/day and +0.054 to +0.072 K/day in the K- and V-band respectively. The uncertainty on the trend is 0.002-0.01 K/day depending on channel. The impact on calibrated T_B is estimated to be less than 0.01 K/day at all channels. Most affected channels are the relative transparent channels, with an estimated drift of ~0.3 K per month. When the effect of the drift is accounted for, the remaining uncertainty (due to the uncertainty on the trend) is ~0.1 K per month.

Information / data	Type / value / equation	Notes / description
Name of effect	Noise diode temperature	
Contribution identifier	A6	
Measurement equation parameter(s) subject to effect	T_N	
Contribution subject to effect (final product or sub-tree intermediate product)	Calibrated T_B	
Time correlation extent & form	Drift	Quasi-systematic
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	PDF peak value increases with time
Uncertainty & units (1σ)	±0.01 K/day	Maschwitz et al., 2013
Sensitivity coefficient	1	
Correlation(s) between affected parameters	A5	Detector non-linearity and noise diode temperature are determined through calibration at the same time
Element/step common for all sites/users?	Yes	
Traceable to …	None	
Validation	Sensitivity study	Maschwitz et al., 2013

5.7 Antenna beam efficiency (A7)

The antenna receiving the scene radiation is characterized by a finite beam and antenna pattern. The power fraction in the sidelobes is estimated by model symulations within 0.1%. Thus, the main beam efficiency η (the ratio of power in the main beam to the total received power) is estimated to be higher than 99.9%. Hewison and Gaffard (2003) estimated η indirectly by comparing calibrations derived from different sets of tip curve angles, and found η increasing from 99.0 to 99.9% with increasing frequency (22 to 30 GHz). The effect of η is accounted for in the calibration. However, there remains an uncertainty affecting the spurious internal radiation entering in the sidelobes, which is estimated within 10% with a resulting T_B effect of less than 0.02 K.

Information / data	Type / value / equation	Notes / description
Name of effect	Antenna beam efficiency	
Contribution identifier	A7	
Measurement equation parameter(s) subject to effect	T_C, T_H	$T_{Heff} = \eta T_H + (1-\eta)T_{Bamb}$ $T_{Ceff} = \eta T_C + (1-\eta)T_{Bamb}$
Contribution subject to effect (final product or sub-tree intermediate product)	Calibrated T_B	
Time correlation extent & form	None	Systematic
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	±0.02 K	Maschwitz et al., 2013
Sensitivity coefficient	1	
Correlation(s) between affected parameters	A11	The antenna beam efficiency is related to the finite beamwidth
Element/step common for all sites/users?	Yes	
Traceable to …	None	
Validation	None	

5.8 Mean radiating temperature (A8)

The atmospheric mean radiative temperature (T_{mr}) is a frequency-dependent parameter entering in the tipping curve calibration method. The tipping curve calibration method requires relatively low opacity and thus it is usually applicable to K-band channels only, though in high-altitude low-pressure conditions may also be applied to lower V-band channels (Maschwitz et al., 2013). T_{mr} is usually estimated from either a climatological mean or a linear regression based on ambient surface temperature (T_{srf}), both derived from prior atmospheric profiles processed with radiative transfer calculations. Regression on T_{srf} is more accurate, with rms ranging from 3.4 to 1.1 K from K- to V-band channels in dry and low pressure conditions (Maschwitz et al., 2013) and up to 3.9 K for K-band channels at standard pressure conditions (Han and Westwater, 2000). For air mass lower than 3 (i.e. elevation angles higher than 19.5°, as usually observed by ground-based MWR), T_{mr} uncertainty impacts for up to 0.3 K on K-band calibration. In the V-band, T_{mr} uncertainty impacts for 1-3 K (Hewison and Gaffard, 2003), though the tipping curve method is usually not used for these channels. For conditions described by Maschwitz et al. (2013), T_{mr} uncertainty impact negligibly the K-band and by ≈ 0.1 K the V-band channels.

Information / data	Type / value / equation	Notes / description
Name of effect	Mean radiative temperature	
Contribution identifier	A8	
Measurement equation parameter(s) subject to effect	T_{mr}	Han and Westwater, 2000
Contribution subject to effect (final product or sub-tree intermediate product)	Calibrated T_B	
Time correlation extent & form	None	Random. The error in estimating T_{MR} depends on atmospheric conditions, thus some correlation with diurnal cycle and season may exist
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	±0.3 K (1σ)	Han and Westwater, 2000
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	N/A	
Validation	Sensitivity study	Han and Westwater, 2000

5.9 Antenna pointing (A9)

The uncertainty in antenna pointing affects the T_B measurements in two aspects: calibration and slant path observations. Calibration through the tipping curve method relies on the knowledge of the elevation angle at which the antenna is pointing. A 1-degree mispointing, due to installation accuracy of zenith direction with respect to the surface normal, can lead to a calibration error of several K. This systematic error is explained by a tilt and can be balanced by averaging measurements of symmetric elevation angle prior to the tipping curve procedure. The correction results in a residual pointing uncertainty of 0.05°. This uncertainty has no effect on the K-band, and results in a ±0.1 K T_B uncertainty in the V-band.

The effect on slant path observations is frequency, elevation angle, and scene dependent. Assuming manufacturers' pointing angle accuracy specifications (0.15°), the effect in the 20-60 GHz range has been quantified through perturbations of radiative transfer simulations for six different atmospheric conditions (from tropical to polar winter) and elevation angle from 5 to 90°. At zenith, the impact is negligible (<0.1 K) at all channels. For opaque V-band channels, the impact is negligible (<0.1 K) at all elevation angles. The impact becomes significant (>0.5 K) for elevation angles lower than 25° and frequency lower than 52 GHz. These channel/angle combinations are normally not used for the atmospheric retrievals.

Information / data	Type / value / equation	Notes / description
Name of effect	Antenna pointing angle	
Contribution identifier	A9	
Measurement equation parameter(s) subject to effect	θ	Observing elevation angle (0.15° pointing uncertainty) Han and Westwater, 2010
Contribution subject to effect (final product or sub-tree intermediate product)	Calibrated T_B	
Time correlation extent & form	None	Random
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	±0.0-0.1 K	Maximum values for typical channel/angle combinations used in retrievals
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	None	
Validation	Perturbation analysis	

5.10 **Atmospheric inhomogeneity (A10)**

Atmospheric inhomogeneity affects the quality of the tipping curve calibration method. Thus, uncertainty of T_B calibrated with tipping curve method increases with increasing atmospheric inhomogeneity. Methods are usually used to reduce this effect, based on quality control screenings and averaging in time and azimuth angle (Han and Westwater, 2000). The remaining effect has been estimated as the standard deviation of T_B over a set of scans, resulting in 0.1–0.2 K for the K-band and 0.3-0.4 K in the V-band (Maschwitz et al., 2013), although this probably overestimates the contribution as it potentially captures other short term random effects. Note that this contribution should not be confused with the impact of atmospheric inhomogeneity on the comparison among different measurement techniques (i.e. contribution to colocation uncertainty, which is treated within GAIA-CLIM Work Package 3). Conversely, here we only refer to the impact of atmospheric inhomogeneity to the quality of the tipping curve calibration method.

Information / data	Type / value / equation	Notes / description
Name of effect	Atmospheric inhomogeneity	
Contribution identifier	A10	
Measurement equation parameter(s) subject to effect	G	Detector gain Maschwitz et al., 2013
Contribution subject to effect (final product or sub-tree intermediate product)	Calibrated T_B	
Time correlation extent & form	None	Random. Since it depends on atmospheric conditions, some correlation with diurnal cycle and season may exist
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	±0.1-0.2 K (1σ) – K-band ±0.3-0.4 K (1σ) – V-band	Han and Westwater, 2010 Maschwitz et al., 2013
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	None	
Validation	Sensitivity study	Maschwitz et al., 2013

5.11 **Finite beam width (A11)**

The MWR antenna is characterized by a finite beam width. As described in A1, the contribution from outside the angular range of two antenna half-power beam widths (HPBW) is negligible. However, the finite beam width affects the effective air mass that the antenna is looking at. This effect can be modeled using a Gaussian-shaped lobe with a width matching twice the HPBW. For typical MWR antenna beam widths (<6°), the impact on calibrated T_B depends on the pointing angle, but it is less than 0.1 K at three air masses (~19.5° elevation) for all channels (Han and Westwater, 2000).

Information / data	Type / value / equation	Notes / description
Name of effect	Atmospheric inhomogeneity	
Contribution identifier	A11	
Measurement equation parameter(s) subject to effect	T_B	Brightness temperature of the effective air mass within the antenna finite beam width
Contribution subject to effect (final product or sub-tree intermediate product)	Calibrated T_B	
Time correlation extent & form	None	Systematic
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	±0.1 K (1σ)	Han and Westwater, 2010
Sensitivity coefficient	1	
Correlation(s) between affected parameters	A7	The antenna beam efficiency is related to the finite beamwidth
Element/step common for all sites/users?	Yes	
Traceable to …	None	
Validation	Sensitivity study	Han and Westwater, 2010

6 Uncertainty Summary

Element identifier	Contribution name	Uncertainty contribution form	Typical value	Traceability level (L/M/H)	random, structured random, quasi-systematic or systematic?	Correlated to? (Use element identifier)
A1	Temperature sensor	Normal	K-band ±0.1 K V-band ±0.2 K	H	random	none
A2	Non-ideal target emissivity	Rectangular	±0.02 K	H	systematic	none
A3	LN2 refractive index	Normal	K-band ±0.7 K V-band ±0.6 K	H	systematic	none
A4	Resonance	Normal	K-band ±0.8 K V-band ±0.3 K	M	quasi-systematic	none
A5	Detector non-linearity	Normal	±0.04 K	M	quasi-systematic	A6
A6	Noise diode temperature	Normal PDF peak value increases with time	±0.01 K/day	L	quasi-systematic	A5
A7	Antenna beam efficiency	Normal	±0.02 K	M	systematic	A11
A8	Mean radiative temperature	Normal	±0.3 K	M	random	none
A9	Antenna pointing angle	Normal	±0.1 K	M	random	none
A10	Atmospheric inhomogeneity	Normal	K-band ±0.2 K V-band ±0.4 K	M	random	none
A11	Finite beam width	Normal	±0.1 K	M	systematic	A7

The contribution of the major uncertainty sources is summarised in the Table above. These contributions are obtained following Han and Westwater (2000), Hewison and Gaffard (2003), Hewison (2006), Maschwitz (2012), and Maschwitz et al. (2013). The two calibration methods (LN2 and tip curve) can be applied in series, the tip curve resulting in a correction to the LN2 coefficients (e.g. the noise diode T_N). Typical atmospheric conditions do not allow the tip curve method to be applicable for V-band channels, so the combination only concerns K-band channels. However, keeping the two methods independent gives the opportunity to detect possible calibration problems (Maschwitz et al. 2013). For the GAIA-CLIM dataset, settings were such that only the LN2 calibration was adopted for all MWR instruments but the one in Lindenberg, for which the tipping curve was used for K-band channels.

Maschwitz et al. 2013 report the total calibration uncertainties of tipping curve and LN2 methods for one particular MWR instrument type (RPG HATPRO). The total calibration uncertainties is given as the sum of the systematic contributions in absolute value:

Tipping curve: $u_{T_B(TIP)} = |u_{T_{MR}}| + |u_p| + |u_{atm}|$

LN2: $u_{T_B(LN2)} = |u_{LN_2}| + |u_{res}| + |u_{hot}| + |u_\alpha|$

where the following uncertainties result from:

$u_{T_{MR}}$	derivation of the mean radiative temperature T_{mr}
u_p	beam pointing
u_{atm}	atmospheric inhomogeneities
u_{LN_2}	refractive index of the LN_2 surface
u_{res}	resonances between the receiver and the LN_2 target
u_{hot}	in-situ hot load measurement
u_{α}	detector non-linearity

Similar results were obtained by Hewison (2006) considering another MWR type (Radiometrics MP3000). However, it must be noted that these contributions are systematic on a single calibration realization, but result in random uncertainty when considering long-term time series with multiple repeated calibrations.
Hewison (2006) also report the random uncertainty of typical T_B when using tipping curve or LN2 calibration methods:

Tipping curve: $$u_{T_B(TIP)} = \sqrt[2]{u_{BB}^2 + u_{atm}^2 + u_{T_{ND}}^2 + u_{rec}^2 + u_{T_{MR}}^2}$$

LN2: $$u_{T_B(LN2)} = \sqrt[2]{u_{BB}^2 + u_{LN2}^2 + u_{T_{ND}}^2 + u_{rec}^2}$$

where the following uncertainties result from:

u_{BB}	black-body noise
u_{atm}	atmospheric noise
$u_{T_{ND}}$	T_{ND} noise and drift
u_{rec}	receiver noise
$u_{T_{MR}}$	T_{MR} noise
u_{LN_2}	LN_2 noise

The resulting T_B uncertainties depend on the channel frequency and the atmospheric conditions through T_B itself. Typical systematic and random uncertainties for K- and V-band channels as derived from Hewison (2006) and Maschwitz et al. (2013) (considering two different types of MWR) are summarized in the table below. All values are in Kelvin. Note that the given uncertainties depend upon atmospheric conditions, e.g. tipping curve uncertainties may increase with increasing atmospheric opacity.

Reference	**MWR type**	**TIP** (K)		**LN2** (K)		
		K-band	V-band	K-band	V-band	
Maschwitz et al. 2013	HATPRO	±0.1-0.2	±0.6-0.7	±0.9-1.6	±0.2-1.0	systematic
Hewison 2006	MP3000	±0.2-0.5	±0.4-0.8	±0.8-1.0	±0.2-1.0	systematic
Hewison 2006	MP3000	±0.3-0.5	±1.5-4.1	±0.6-1.1	±0.1-0.6	random

7 Traceability uncertainty analysis

Traceability level definition is given in Table 2.

Table 2. Traceability level definition table

Traceability Level	Descriptor	Multiplier
High	SI traceable or globally recognised community standard	1
Medium	Developmental community standard or peer-reviewed uncertainty assessment	3
Low	Approximate estimation	10

Analysis of the summary table would suggest the following contributions, shown in Table 3, should be considered further to improve the overall uncertainty of the MWR brightness temperature product. The entries are given in an estimated priority order.

Table 3. Traceability level definition further action table.

Element identifier	Contribution name	Uncertainty contribution form	Typical value	Traceability level (L/M/H)	random, structured random, quasi-systematic or systematic?	Correlated to? (Use element identifier)
A4	Resonance	Normal	K-band ±0.8 K V-band ±0.3 K	M	quasi-systematic	none
A6	Noise diode temperature	Normal PDF peak value increases with time	±0.01 K/day	L	quasi-systematic	A5
A3	LN2 refractive index	Normal	K-band ±0.7 K V-band ±0.6 K	H	systematic	none

7.1 Recommendations

The top priority is to reduce the resonance contribution (A4). This requires technological improvements (e.g. anti-reflection coating of cold calibration target) which have been already developed and exploited on newer generation commercial MWR instruments.

The second priority is to better characterise the noise diode temperature drift (A6). This has been only estimated for one instrument during one field experiment. Ideally it should be characterized for each instrument periodically to account for drifts within two LN2 calibrations.

The third priority requires new and more accurate laboratory measurement of LN2 refractive index (A3), in order to update the uncertainty achievable by Benson et al., 1983.

In addition, although the contribution from the non-ideal target emissivity (A2) is deemed to be small, the lack of MW radiometry standards is currently hampering the SI traceability of MWR observations. The U.S. National Institute of Standard and Technologies (NIST) is currently developing such standards for MW radiometry (Houtz et al., 2016). NIST plans to be able to provide SI-traceability for calibration targets and transfer standards in the next few years.

8 Conclusion

The MWR brightness temperature product has been assessed against the GAIA CLIM traceability and uncertainty criteria.

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Product Traceability and Uncertainty for the Microwave Radiometer (MWR) temperature profile product

Version 1.0

GAIA-CLIM
Gap Analysis for Integrated
Atmospheric ECV Climate Monitoring
Mar 2015 - Feb 2018

A Horizon 2020 project; Grant agreement: 640276

Date: 30 November 2017

Dissemination level: PU

Work Package 2; Task 2.1.2; Complied by Domenico Cimini (CNR)

Consiglio Nazionale delle Ricerche

Table of Contents

Version history

Version	Principal updates	Owner	Date
0.1 draft	First draft – adapted existing text to the template provided by NPL	CNR	28.06.2017
0.2 draft	Second draft – Sent for initial external comments	CNR	30.06.2017
0.3 draft	Third draft – after external comments from Paul Green (NPL)	CNR	27.07.2017
0.4 draft	Fourth draft – after Webex meeting on Oct 9th 2017	CNR	8.11.2017
1.0	First issue as annex F of D2.6	CNR	30.11.2017

1 Product overview

Product name: MWR temperature profile product
Product technique: Temperature profile retrieval from multichannel brightness temperature measurements and a priori knowledge
Product measurand: Temperature [K]
Product form/range: Profile
Product dataset: TOPROF data set
Site/Sites/Network location:

SITE	LAT	LON	HEIGHT(m)	MWR	LOCATION	COUNTRY
JOYCE	50.91	6.41	111	HATPRO G2	Juelich	DE
LACROS	51.35	12.43	125	HATPRO G2	Liepzig	DE
Payerne	46.82	6.95	491	HATPRO G1	Payerne	CH
SIRTA	48.80	2.36	156	HATPRO G2	Paris	FR
CESAR	51.97	4.93	-0.7	HATPRO G1	Cabauw	NL
RAO	52.21	14.12	125	MP3000A	Lindenberg	DE

Product time period: Jan 1, 2015 – Feb 27, 2016
Data provider: TOPROF
Instrument provider: Site management
Product assessor: Domenico Cimini, CNR
Assessor contact email: domenico.cimini@imaa.cnr.it

1.1 Guidance notes

For general guidance see the Guide to Uncertainty in Measurement & its Nomenclature, published as part of the GAIA-CLIM project.

This document is a measurement product technical document which should be stand-alone i.e. intelligible in isolation. Reference to external sources (mostly peer-reviewed) and documentation from previous studies is given, but the content provided here shall not require the reading of all these reference documents to gain a clear understanding of the GAIA CLIM product and associated uncertainties entered into the Virtual Observatory (VO).

In developing this guidance, we adopted the convention proposed by the QA4ECV project (http://www.qa4ecv.eu/) through the Traceability and Uncertainty Propagation Tool (TUPT). This convention is summarized in Figure 1.

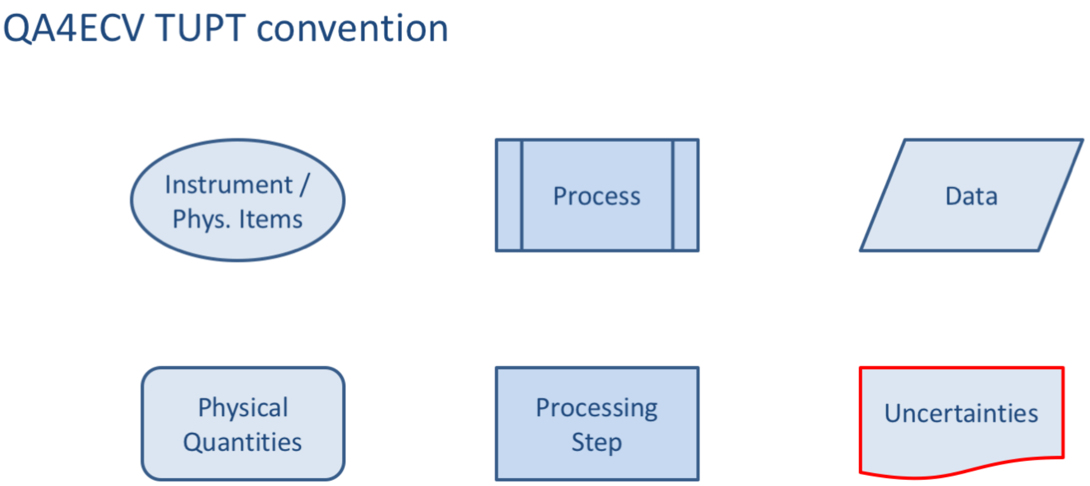

Figure 1. The convention proposed by the QA4ECV project (http://www.qa4ecv.eu/) through the Traceability and Uncertainty Propagation Tool (TUPT). This convention is adopted hereafter to draw the MWR model diagram.

The contribution table to be filled for each traceability contributor has the form seen in Table 1.

Table 1. The contributor table.

Information / data	Type / value / equation	Notes / description
Name of effect		
Contribution identifier		
Measurement equation parameter(s) subject to effect		
Contribution subject to effect (final product or sub-tree intermediate product)		
Time correlation extent & form		
Other (non-time) correlation extent & form		
Uncertainty PDF shape		
Uncertainty & units		
Sensitivity coefficient		
Correlation(s) between affected parameters		
Element/step common for all sites/users?		
Traceable to …		
Validation		

Name of effect – The name of the contribution. Should be clear, unique and match the description in the traceability diagram.

Contribution identifier - Unique identifier to allow reference in the traceability chains.

Measurement equation parameter(s) subject to effect – The part of the measurement equation influenced by this contribution. Ideally, the equation into which the element contributes.

Contribution subject to effect – The top level measurement contribution affected by this contribution. This can be the main product (if on the main chain), or potentially the root of a side branch contribution. It will depend on how the chain has been sub-divided.

Time correlation extent & form – The form & extent of any correlation this contribution has in time.

Other (non-time) correlation extent & form – The form & extent of any correlation this contribution has in a non-time domain. For example, spatial or spectral.

Uncertainty PDF shape – The probability distribution shape of the contribution, Gaussian/Normal Rectangular, U-shaped, log-normal or other. If the form is not known, a written description is sufficient.

Uncertainty & units – The uncertainty value, including units and confidence interval. This can be a simple equation, but should contain typical values.

Sensitivity coefficient – Coefficient multiplied by the uncertainty when applied to the measurement equation.

Correlation(s) between affected parameters – Any correlation between the parameters affected by this specific contribution. If this element links to the main chain by multiple paths within the traceability chain, it should be described here. For instance, SZA or surface pressure may be used separately in a number of models & correction terms that are applied to the product at different points in the processing.

Element/step common for all sites/users – Is there any site-to-site/user-to-user variation in the application of this contribution?

Traceable to – Describe any traceability back towards a primary/community reference.

Validation – Any validation activities that have been performed for this element?

2 Introduction

This document presents the Product Traceabililty and Uncertainty (PTU) information for the Microwave Radiometer (MWR) temperature profile product. The aim of this document is to provide supporting information for the users of this product within the GAIA-CLIM VO.

Using the convention in Figure 1, the main chain of the MWR instrument is pictured in Figure 2. The red boxes indicates the two main processes:
A) Calibration: the conversion from raw voltages corresponding to the received atmospheric

radiance into calibrated brightness temperature (T_B);
B) Inversion: the inversion of calibrated T_B with the combination of some a priori knowledge to estimate the atmospheric products (retrievals).

Thus, MWR uncertainties are divided in two groups: those affecting the MWR calibration (i.e. from atmospheric radiance to calibrated T_B) and those affecting the retrieval method (from calibrated T_B to MWR retrievals). The parent document (GAIA-CLIM PTU document for MWR brightness temperature product) treats the calibration process (A) and the contributions to the T_B uncertainty. This document treats the inversion process (B) and how the T_B uncertainty combine with other uncertainty sources to contribute to the uncertainty of the retrieved temperature profile.

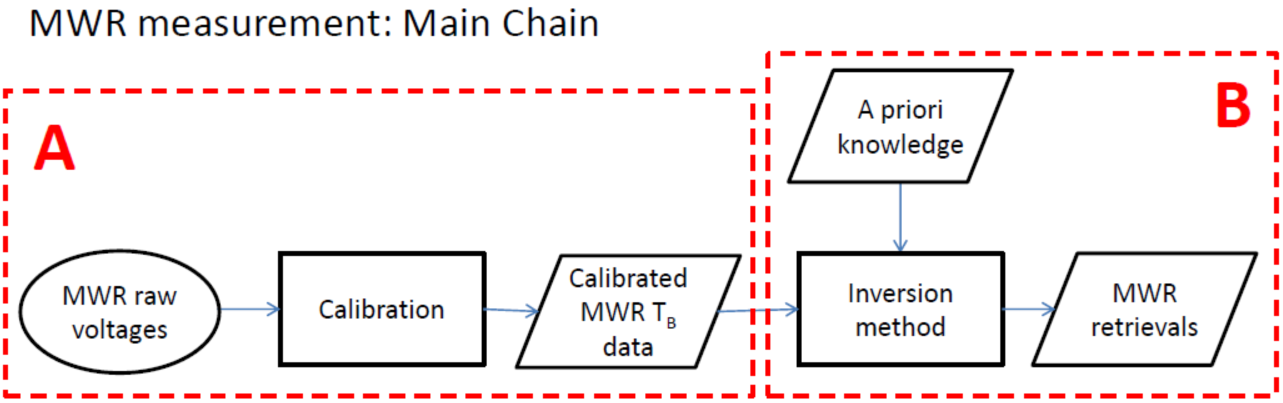

Figure 2. The main chain of the MWR instrument model diagram. The main chain displays the process of producing a geophysical product from the MWR instrument measurements. The process A (from raw voltages to calibrated brightness temperature Tb) is treated in this document. The process B is treated in three children documents.

3 Instrument description

Ground-based microwave radiometers (MWR) are instruments calibrated to measure the natural down-welling thermal emission from the atmosphere. The quantity measured by a MWR is atmospheric radiance [$W/(m^2 \cdot sr \cdot Hz)$], which is typically converted into brightness temperature (T_B, [K]) to adopt more familiar units.

Atmospheric temperature and humidity profiles, as well as column-integrated Total Water Vapour Content (TWVC) and Total Liquid Water Content (TLWC), can be inferred from ground-based MWR T_B observations.

Review articles on MWR measurements are given by Westwater et al., 2004 & 2005. Common MWR commercial units operate several channels in the 20-60 GHz frequency range. The 20-30 GHz range is referred to as K-band, while the 50-60 GHz range is called V-band.

Figure 3 provides details of the MWR measurement metrological model chain for the inversion process (B). It describes the flow diagram from the a priori knowledge and the calibrated T_B, including uncertainty sources (highlighted in red), to the retrieved atmospheric temperature product.

The uncertainty of the inverse method, that is the analysis algorithm to transform the calibrated T_B into the atmospheric products, contributes to the total uncertainty affecting the MWR atmospheric products. A variety of methods are currently used to solve the inverse problem, with somewhat different implementations, and their performances have been compared to some degree (Solheim et al. 1998; Cimini et al., 2006). Statistical algorithms, including multivariate statistical regression and neural networks, are usually exploited as they are suitable to be applied in real time. Conversely, physical retrieval methods, such as optimal estimation methods (OEM), are computationally more expensive as they solve the inverse problem in a physically consistent way. OEM optimally couples MWR observations with a priori background knowledge, accounting for uncertanity from both the observations and background and propagating uncertainty to the final product. An estimate of the uncertainty on the retrieved profiles can be derived by assuming the errors are normally distributed about the solution and that the problem is only moderately non-linear (Rodgers, 2000).

The OEM retrieval method is affected by instrumental uncertainty (detailed in the parent document GAIA-CLIM PTU document for MWR brightness temperature product) as well as other sources of uncertainty, such as a priori, absorption model, spectral response function, profile discretization, smoothing and representativeness errors (Hewison, 2006; Cimini et al., 2010; Stähli et al., 2013).

For the OEM, we adopt the following notation:

$\mathbf{y}$	the measurement vector
$\mathbf{y}_0$	the mean measurement vector
$\mathbf{x}$	the atmospheric state vector (in this case, the temperature profile)
$\mathbf{x}_b$	the background (a priori) atmospheric state vector
$\hat{\mathbf{x}}$	the estimated atmospheric state vector
$\mathbf{K}$	the Jacobian matrix of the observation vector with respect to the state vector
$\mathbf{B}$	the background (a priori) uncertainty covariance matrix
$\mathbf{R}$	the measurement uncertainty covariance matrix
$u(\hat{\mathbf{x}})$	the estimated retrieval uncertainty affecting $\hat{\mathbf{x}}$

Thus, the OEM provides the following iterative solution (Rodgers, 2000):

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

While the estimated retrieval uncertainty is given by the diagonal terms of the posterior covariance matrix:

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

Inaccurate estimates of **R** and **B** would cause the OEM to produce results that are not strictly optimal. Given the relative larger uncertainty associated with the estimation of the background error covariances, this is likely to be the dominant source of non-optimality (Hewison, 2006).

4 Product Traceability Chain

MWR temperature profile product

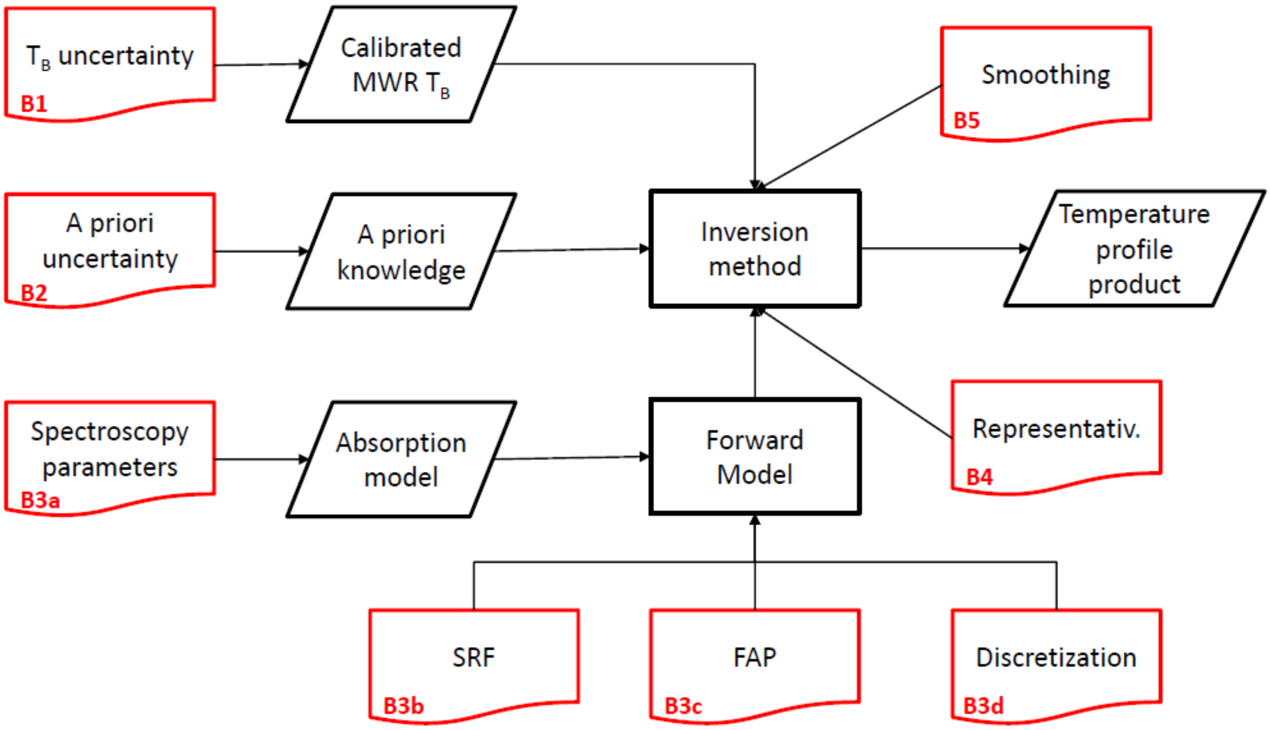

Figure 3. The metrological model chain of the MWR temperature profile product. It describes the flow diagram of the measurement, from the a priori knowledge and the calibrated TB, including uncertainty sources (highlighted in red), to the retrieved atmospheric temperature product.

All uncertainties quoted here are in the point-to-point profile temperature product at vertical spacing of the retrievals (~20-350 m within 0-5 km; 350-700 m within 5-10 km).

5 Element contributions

5.1 Brightness temperature uncertainty (B1)

The primary measurand of a MWR is brightness temperature (T_B). The estimated uncertainty for the measured T_B are detailed in the parent document GAIA-CLIM PTU document for MWR brightness temperature product. The T_B uncertainty are then propagated through the OEM formalism to estimate the uncertainty of the retrieved temperature profile. As shown in **Error! Reference source not found.** (right), the typical T_B uncertainty of 0.3-1.1 K maps to typical uncertainty contributions of 0.2-0.3 K within the lowest 2 km and with less than 0.2 K above 2 km.

Information / data	Type / value / equation	Notes / description
Name of effect	T_B uncertainty	
Contribution identifier	B1	
Measurement equation parameter(s) subject to effect	**R**	
Contribution subject to effect (final product or sub-tree intermediate product)	$\hat{\mathbf{x}} \pm u(\hat{\mathbf{x}})$	Estimated temperature profile and uncertainty
Time correlation extent & form	None	Random
Other (non-time) correlation extent & form	None	Random
Uncertainty PDF shape	Normal	
Uncertainty & units	<0.3 K (1σ) below 2 km <0.2 K (1σ) above 2 km	Point to point uncertainties at retrieval vertical resolution
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	None	
Validation	Field experiments	Maschwitz et al., 2013

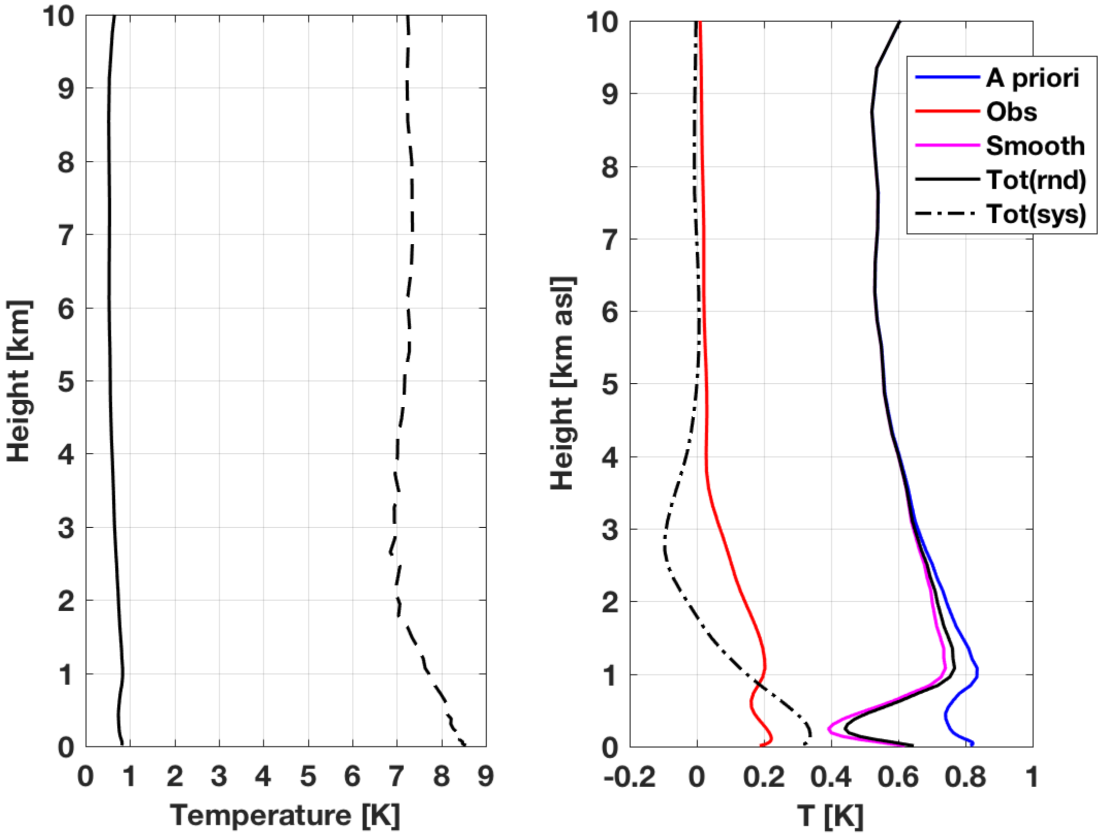

Figure 4. Left: Typical uncertainty for the a priori background from NWP (solid) and climatology (dashed). NWP data from Martinet et al, 2015. Climatology data courtesy of DWD (computed from radiosonde launched from Lindenberg in 2003-2004). Right: Contribution from a priori NWP (blue), observation (red), smoothing (magenta) uncertainties to the total uncertainty (black solid). The systematic uncertainty estimated for MWR calibration is shown in black dash-dotted line.

5.2 A priori uncertaity (B2)

When the Optimal Estimation Method is used, MWR observations are optimally coupled with a priori background knowledge, accounting for the uncertainty from both the observations and the background. Thus, an estimate of the a priori background uncertainty is needed, in the form of the background error covariance matrix **B**. A priori information may come from different sources, usually climatology (e.g. a set of historic radiosonde profiles) or the output of a numerical weather prediction (NWP) model. In case of climatology, **B** is estimated as the covariance matrix with respect to the mean value. In case of NWP model output, **B** is estimated from an ensemble of perturbed assimilation cycles (Martinet et al., 2015), similar to / the same as that used operationally for data assimilation purposes. **Error! Reference source not found.** shows examples of two such a priori uncertainties. However, the operational **B** matrix was found to significantly underestimate the NWP error for planetary boundary layer temperature above complex terrain (Martinet et al., 2017) and polar regions (Cimini et al. 2010). Thus, in those cases the diagonal terms of the temperature **B** matrix were modified below 2 km altitude considering the variance of typical radiosonde minus NWP differences. This correction resulted in a multiplicative factor of ~2-3 in std.

Information / data	Type / value / equation	Notes / description
Name of effect	A priori uncertainty	
Contribution identifier	B2	

Measurement equation parameter(s) subject to effect	**B**	
Contribution subject to effect (final product or sub-tree intermediate product)	$\hat{\mathbf{x}} \pm u(\hat{\mathbf{x}})$	Estimated temperature profile and uncertainty
Time correlation extent & form	None	Random
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	0.4-0.7 K (1σ)	Martinet et al., 2015
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	None	
Validation	Field experiment	Martinet et al., 2017

5.3 Forward Model (B3)

Any inversion method relying on Forward Model (FM) calculations, such as OEM, is affected by the uncertainty of the assumed model. The FM uncertainty includes uncertainty related to the atmospheric absorption model spectroscopy, the fast model parametrization, and the profile representation in the radiative transfer model. The contributions of these terms to the overall forward model error covariance have been evaluated by Hewison (2006), showing it is dominated by the uncertainties in the spectroscopy, which are the most difficult to estimate accurately.

Information / data	Type / value / equation	Notes / description
Name of effect	Profile discretization	
Contribution identifier	B3	
Measurement equation parameter(s) subject to effect		
Contribution subject to effect (final product or sub-tree intermediate product)	$\hat{\mathbf{x}} \pm u(\hat{\mathbf{x}})$	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	<0.2 K (1σ) below 3 km <0.1 K (1σ) above 3 km	Based on Hewison, 2006
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	None	
Validation	None	On-going

5.4 Spectroscopic parameters (B3a)

The radiative transfer model (RTM) calculations are affected by the uncertainty of the assumed atmospheric absorption model. This relates to the uncertainty affecting the values of the spectroscopic parameters used within the model. This contribution is often estimated as the difference in zenith T_B calculated by two or more different absorption models (Hewison, 2006; Cimini et al., 2010). Estimates for a global average are reported in the table below (after Hewison, 2006; Table 2-1). These values map onto an uncertainty for the temperature profile of the order of 0.1-0.2 K in the first 3 km and below 0.1 K above that.

ν[GHz]	22.235	23.035	23.835	26.235	30.00	51.250	52.280	53.850	54.940	56.660	57.290	58.800
σT_B[K]	1.01	1.01	0.94	0.74	0.69	1.20	0.88	0.23	0.03	0.01	0.01	0.01

Another approach consists in quantifying the spectroscopic uncertainty impact by perturbing the atmospheric profile by an amount that is reasonably attributable to the spectroscopic uncertainty (Stähli et al., 2013). However, a rigorous approach requires propagating uncertainties in line parameters to uncertainty in absorption, as suggested by Boukabara et al. 2005. Such a rigourous approach is currently being investigated within GAIA-CLIM (Cimini, 2017).

Information / data	Type / value / equation	Notes / description
Name of effect	Spectroscopic parameters	
Contribution identifier	B3a	
Measurement equation parameter(s) subject to effect	$\mathbf{S}_i$	
Contribution subject to effect (final product or sub-tree intermediate product)	B3	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	<0.2 K (1σ) below 3 km <0.1 K (1σ) above 3 km	Based on Hewison, 2006
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	None	
Validation	None	On-going

5.5 Spectral Response Function (B3b)

RTM calculations require the knowledge of the channel spectral response function (SRF), which characterizes the finite bandwidth for each MWR channel (Löhnert and Maier, 2012). Band-averaged T_B can be obtained by convolving the SRF with high-resolution RTM calculations. Band-averaged T_B may significantly differ from monochromatic T_B evaluated at the channel's center frequency, as the atmospheric absorption may change non-linearly across the bandwidth of each channel. To avoid the need for expensive multiple RTM computations, it is often assummed to be approximated by an equivalent monochromatic frequency (EMF) for each channel (Cimini et al., 2010). The EMF is determined as the monochromatic frequency that minimizes the difference with the band-averaged T_B for a representative data set of atmospheric profiles. The EMF does not always correspond to the nominal central frequency. Once the EMF is accurately determined, the impact on T_B is negligible (i.e. < 0.05 K, Cimini et al., 2006; Hewison, 2006).

Information / data	Type / value / equation	Notes / description
Name of effect	Spectral Response Function (SRF)	
Contribution identifier	B3b	
Measurement equation parameter(s) subject to effect	$\boldsymbol{S}_i$	
Contribution subject to effect (final product or sub-tree intermediate product)	B3	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	<0.1 K (1σ)	
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	None	
Validation	Field experiments	Cimini et al., 2006 Hewison et al., 2006

5.6 Fast Absoption Predictor (B3c)

The OEM solution introduced in Section 3 requires iterative calculations. Thus, a fast RTM is mostly convenient, using a Fast Absorption Predictor (FAP) model to calculate the atmospheric absorption as a function of thermodynamical predictors (Hewison, 2006). One such fast RTM is RTTOV-gb, developed specifically for ground-based MWR observations (De Angelis, 2016). RTTOV-gb has been tested against reference RTM, showing residual errors smaller than typical MWR T_B uncertainties (<0.05 K for K-band channels, 0.01-0.2 K for V-band channels; 1σ at 19°-90° elevation). These values are a factor ~2-3 smaller than those reported by Hewison, 2006 (Table 2-3). This is probably due to the choice of better-suited predictors, which in RTTOV-gb follows the ones carefully developed for satellite RTM calculations.

Information / data	Type / value / equation	Notes / description
Name of effect	Fast Absoption Predictor (FAP)	
Contribution identifier	B3c	
Measurement equation parameter(s) subject to effect	$\mathbf{S}_i$	
Contribution subject to effect (final product or sub-tree intermediate product)	B3	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	<0.1 K (1σ)	
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	None	
Validation	Numerical validation	De Angelis et al., 2016

5.7 Discretization (B3d)

The discretization of the background profiles introduces uncertainty in T_B calculated by the RTM. This contribution has been evaluated using a set of high-resolution radiosondes to compute T_B through a RTM and comparing with T_B calculated using the same profiles reduced by a discretization method, as that used for NWP models (Hewison, 2006; Table 2-4). Large impact is found when using WMO standard levels (0.4-1.7 K), which reduces substantially when significant levels are added (0.03-0.21 K). Using the levels designed for RTTOV-gb (De Angelis et al., 2016), the impact on T_B becomes negligible (<0.05 K).

Information / data	Type / value / equation	Notes / description
Name of effect	Discretization	
Contribution identifier	B3d	
Measurement equation parameter(s) subject to effect	$\mathbf{S}_i$	
Contribution subject to effect (final product or sub-tree intermediate product)	B3	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	<0.1 K (1σ)	
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	None	
Validation		Using standard atmosphere and RTTOV-gb levels (De Angelis et al., 2016)

5.8 Representativeness (B4)

The representativeness error accounts for the instrument sensitivity to fluctuations on smaller scales than can be represented by the background. To compensate for this, it is usual to add the representativeness errors to the instrumental error to get a larger observational error. The representativeness error has been estimated by studying the fluctuations in the MWR signal on typical time scales within a 6-day period of clear and cloudy conditions (Hewison, 2006). It was found that the representativeness term evaluated in this way dominates the observation error of those channels most sensitive to cloud. These values map onto an uncertainty for the temperature profile of the order of 0.1-0.3 K in the first 3 km and below 0.1 K above that. Ideally, the representativeness error shall be evaluated dynamically, e.g. based on time series of observations within 1 hour window of each observation. This would allow the errors to be reduced in periods of atmospheric stability, when MWR observations are more representative of the background state. Inclusion of observations of meteorological covariates would help better quanify this uncertainty, although this is not currently performed.

Information / data	Type / value / equation	Notes / description
Name of effect	Representativeness error	
Contribution identifier	B4	
Measurement equation parameter(s) subject to effect	**R**	
Contribution subject to effect (final product or sub-tree intermediate product)	$\hat{\mathbf{x}} \pm u(\hat{\mathbf{x}})$	
Time correlation extent & form	diurnal/seasonal	Depends on atmospheric conditions, and thus may be correlated with diurnal/seasonal cycle
Other (non-time) correlation extent & form	None	
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	<0.3 K (1σ) below 3 km <0.1 K (1σ) above 3 km	Based on Hewison, 2006
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	None	
Validation	None	

5.9 Smoothing error (B5)

The smoothing error is part of the total uncertainty estimated with the OEM. It is related to the vertical resolution of MWR temperature profiles, which is limited due to the passive approach. A quantitative definition of the vertical resolution builds on the averaging kernel matrix concept. The averaging kernel defines the sensitivity of the retrieved quantities to the true atmospheric state. The broadness of the averaging kernels gives information on the vertical resolution; e.g. a perfect vertical resolution corresponds to averaging kernels in the form of delta functions. Using the same notation as in Section 3, the averaging kernel matrix is defined as (Rodgers, 2000):

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

The smoothing error is defined as $(\mathbf{A}-\mathbf{I})(\mathbf{x}-\mathbf{x_b})$ whose covariance is $\mathbf{S}_{\mathrm{S}} = (\mathbf{A}-\mathbf{I})\mathbf{B}(\mathbf{A}-\mathbf{I})^T$. As shown in **Error! Reference source not found.** (right), the smoothing error is dominating the total uncertainty.

Information / data	Type / value / equation	Notes / description
Name of effect	Smoothing error	
Contribution identifier	B5	
Measurement equation parameter(s) subject to effect	$\mathbf{S}_{\mathrm{i}}$	
Contribution subject to effect (final product or sub-tree intermediate product)	$\hat{\mathbf{x}} \pm u(\hat{\mathbf{x}})$	
Time correlation extent & form	None	
Other (non-time) correlation extent & form	Vertical	The averaging kernels indicate the correlation of the retrievals at different vertical levels.
Uncertainty PDF shape	Normal	
Uncertainty & units (1σ)	0.4-0.8 K (1σ) from 0-10 km	
Sensitivity coefficient	1	
Correlation(s) between affected parameters	None	
Element/step common for all sites/users?	Yes	
Traceable to …	OEM formalism	Traceable linked to that of **B** and **R**
Validation	Field experiments	Löhnert and Maier, 2012

6 Uncertainty Summary

Element identifier	Contribution name	Uncertainty contribution form	Typical value	Traceability level (L/M/H)	random, structured random, quasi-systematic or systematic?	Correlated to? (Use element identifier)
B1	T_B uncertainty	Normal	0.3 K	M	random	None
B2	A priori	Normal	0.4-0.7 K	M	random	None
B3	Forward model	Normal	0.2 K	M	random	None
B3a	Spectroscopy	Normal	0.2 K	L	random	None
B3b	SRF	Normal	<0.1 K	H	systematic	None
B3c	FAP	Normal	<0.1 K	H	random	None
B3d	Discretization	Normal	<0.1 K	H	systematic	None
B4	Representativeness	Normal	0.1-0.3 K	L	random	None
B5	Smoothing	Normal	0.4-0.8 K	H	random	None

The estimated uncertainties are combined following the OEM formalism (Rodgers, 2000). Using the same notation as in Section 3, the random uncertainty of the estimated temperature profile $\hat{\mathbf{x}}_i$ is given by the diagonal terms of the posterior covariance matrix:

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

The background uncertainty covariance matrix (**B**) and the measurement uncertainty covariance matrix (**R**) are related to the Uncertainty Summary Table above as follows. **B** is given by the a priori uncertainty (B2). **R** is usually split in three contributions **R** = **E** + **F** + **M** (Hewison, 2006), where the instrument noise (**E**) corresponds to T_B uncertainty (B1); **F** corresponds to the forward model uncertainty (B3); and **M** corresponds to the representativeness uncertainty (B4). The smoothing uncertainty (B5) is given by the combined contributions of **B**, **R**, and $\mathbf{K}_i$ as explained in Section 5.9. The relative contributions of **B**, **R**, and smoothing to the total random uncertainty are depicted in Figure 4.

Introducing the gain matrix $\mathbf{G} = \mathbf{S}_i\mathbf{K}_i^{\mathrm{T}}\mathbf{R}^{-1}$ (Rodgers, 2000), the systematic uncertainty of the retrieved temperature profile is estimated in the assumption of a linear retrieval as:

$$u_{sys}(\hat{\mathbf{x}}_i) = \mathbf{G} * u_{sys}(\boldsymbol{y})$$

where $u_{sys}(\boldsymbol{y})$ includes the T_B systematic uncertainty affecting the MWR calibration (see the parent GAIA-CLIM PTU document for MWR brightness temperature product). Typical values of the estimated systematic uncertainty are shown in Figure 4. Finally, Figure 5 shows an example of a MWR retrieved temperature profile with the associated random and systemetic uncertainties.

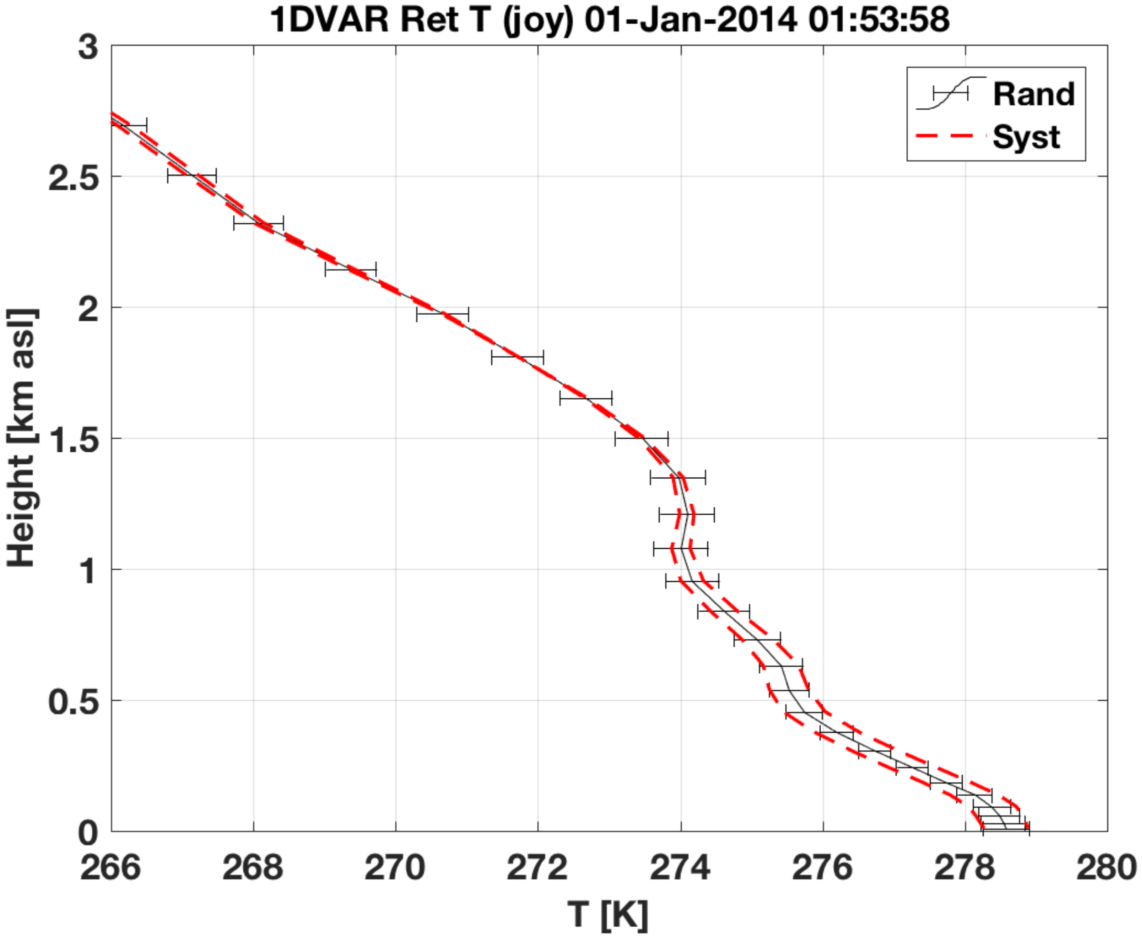

Figure 5. An example of temperature profile retrieval at the Joyce site (Juelich, Germany) on January 1st 2014, 01:53 UTC. The associated random (errorbars) and systematic (red dashed lines) uncertainties are also shown.

7 Traceability uncertainty analysis

Traceability level definition is given in Table 2.

Table 2. Traceability level definition table

Traceability Level	Descriptor	Multiplier
High	SI traceable or globally recognised community standard	1
Medium	Developmental community standard or peer-reviewed uncertainty assessment	3
Low	Approximate estimation	10

Analysis of the summary table would suggest the following contributions, shown in Table 3, should be considered further to improve the overall uncertainty of the MWR temperature profile product. The entries are given in an estimated priority order.

Table 3. Traceability level definition further action table.

Element identifier	Contribution name	Uncertainty contribution form	Typical value	Traceability level (L/M/H)	random, structured random, quasi-systematic or systematic?	Correlated to? (Use element identifier)
B3a	Spectroscopy	Normal	0.2 K	L	random	None
B2	A priori	Normal	0.4-0.7 K	M	random	None
B4	Representativeness	Normal	0.1-0.3 K	L	random	None

7.1 Recommendations

Suggestions for improving the assessment of the T_B calibration uncertainty (B1) are given in the parent document GAIA-CLIM PTU document for MWR brightness temperature product.

In addition, the top priority is to quantify rigorously the spectroscopic parameter contribution (B3a), which may be significantly underestimated. This is ongoing within GAIA-CLIM (Cimini, 2017).

Another priority is to better characterise the a priori uncertainty (B2), especially when the a priori information is from a NWP model. There is emerging evidence that this contribution may be underestimated for sites with strong surface temperature inversions (Cimini et al., 2010; Martinet et al., 2017).

Finally, the representativeness error (B4) shall be characterised for each site and MWR instrument. Inclusion of observations of meteorological covariates would help better quanify this uncertainty. Ideally, this could be evaluated dynamically to make this contribution flow-dependent.

8 Conclusion

The MWR temperature profile product has been assessed against the GAIA CLIM traceability and uncertainty criteria.

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