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.

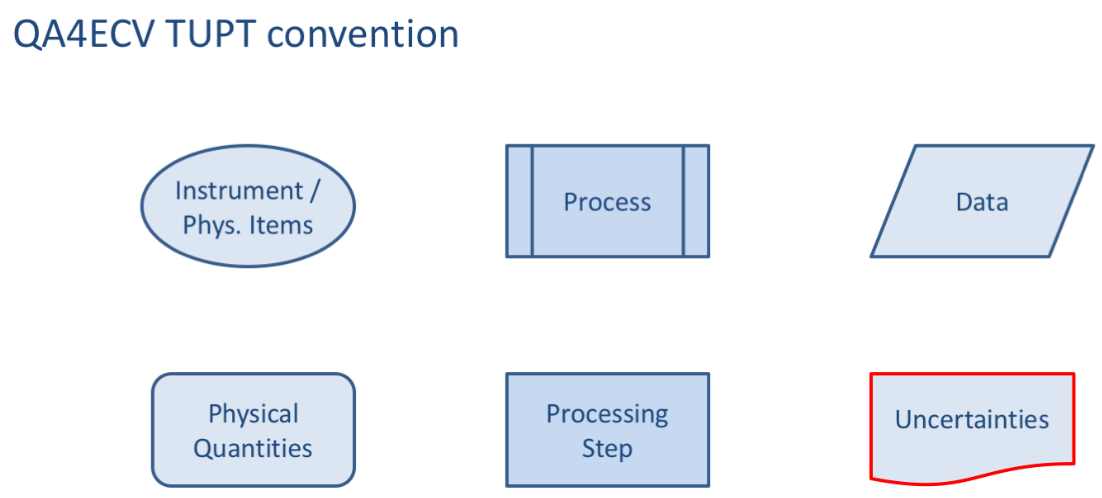

Figure 1. The convention proposed by the QA4ECV project (http://www.qa4ecv.eu/) through the Traceability and Uncertainty Propagation Tool (TUPT). This convention is adopted hereafter to draw the MWR model diagram.

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.

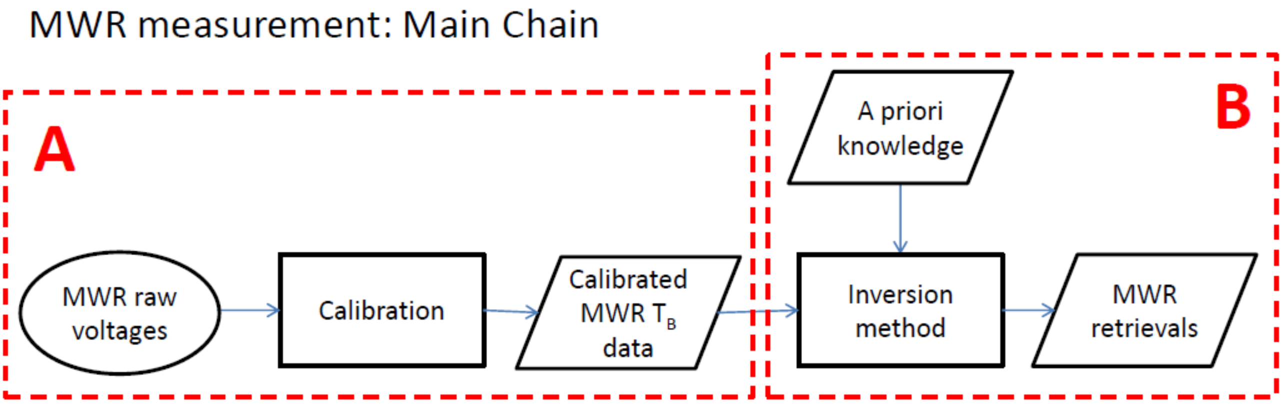

Figure 2. The main chain of the MWR instrument model diagram. The main chain displays the process of producing a geophysical product from the MWR instrument measurements. The process A (from raw voltages to calibrated brightness temperature Tb) is treated in this document. The process B is treated in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

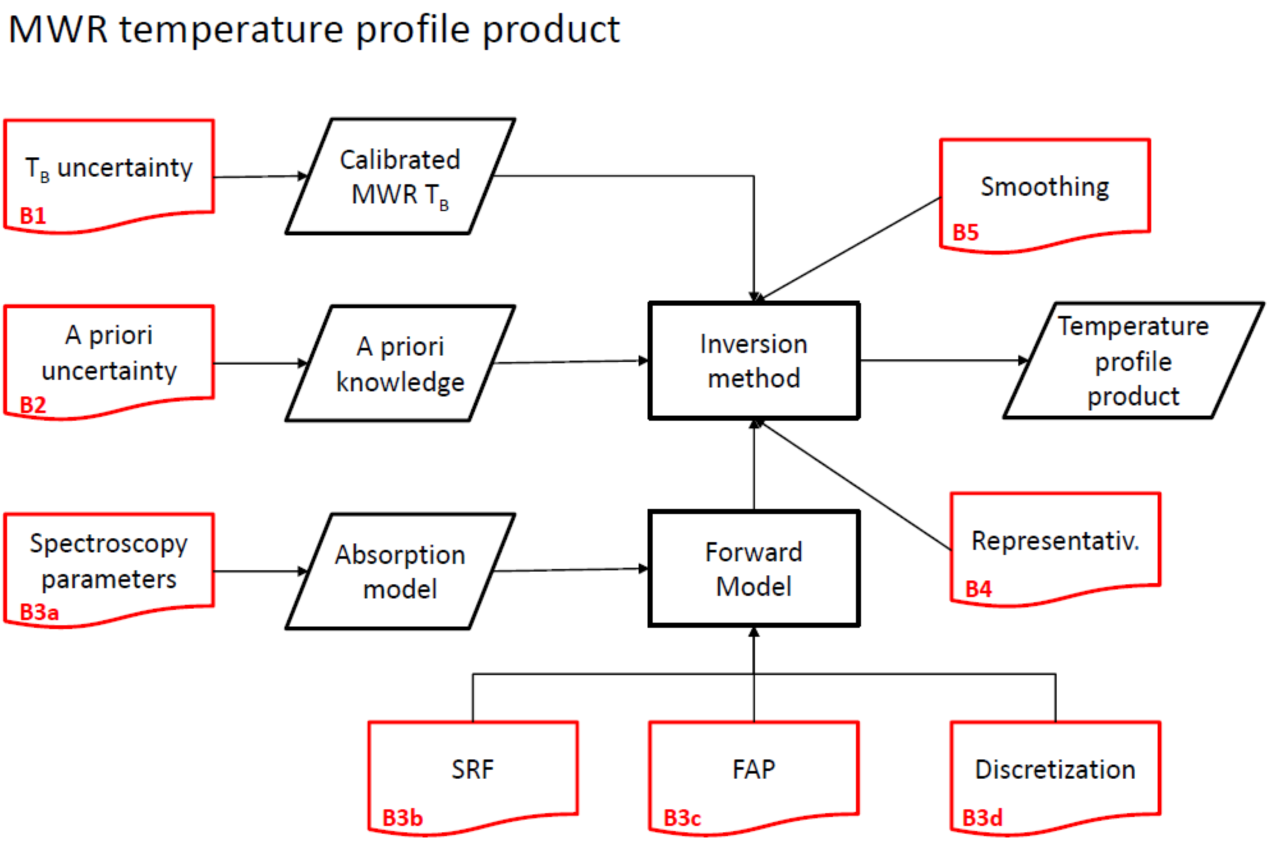

Figure 3. The metrological model chain of the MWR temperature profile product. It describes the flow diagram of the measurement, from the a priori knowledge and the calibrated TB, including uncertainty sources (highlighted in red), to the retrieved atmospheric temperature product.

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

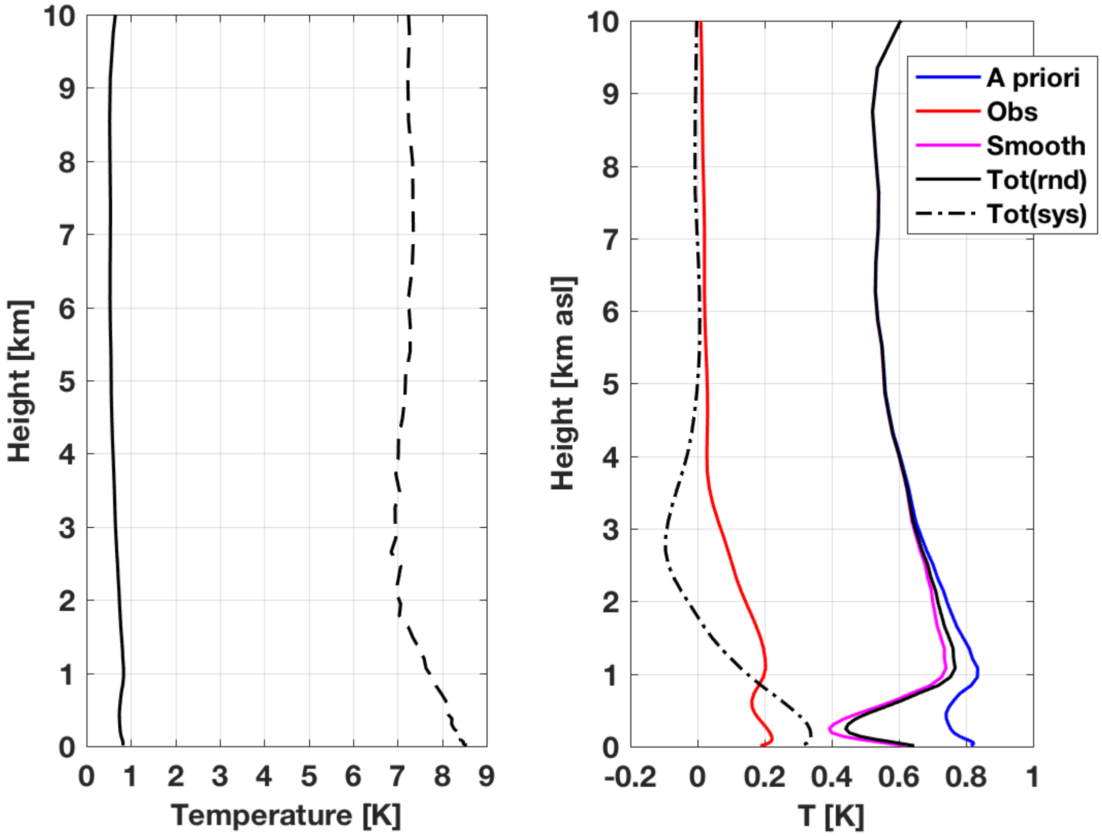

Figure 4. Left: Typical uncertainty for the a priori background from NWP (solid) and climatology (dashed). NWP data from Martinet et al, 2015. Climatology data courtesy of DWD (computed from radiosonde launched from Lindenberg in 2003-2004). Right: Contribution from a priori NWP (blue), observation (red), 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:

$$u_{rnd}(\hat{\mathbf{x}}_i) = \mathbf{diag}(\mathbf{S}_i) = \mathbf{diag}([\mathbf{B}^{-1} + \mathbf{K}_i^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{K}_i]^{-1})$$

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.

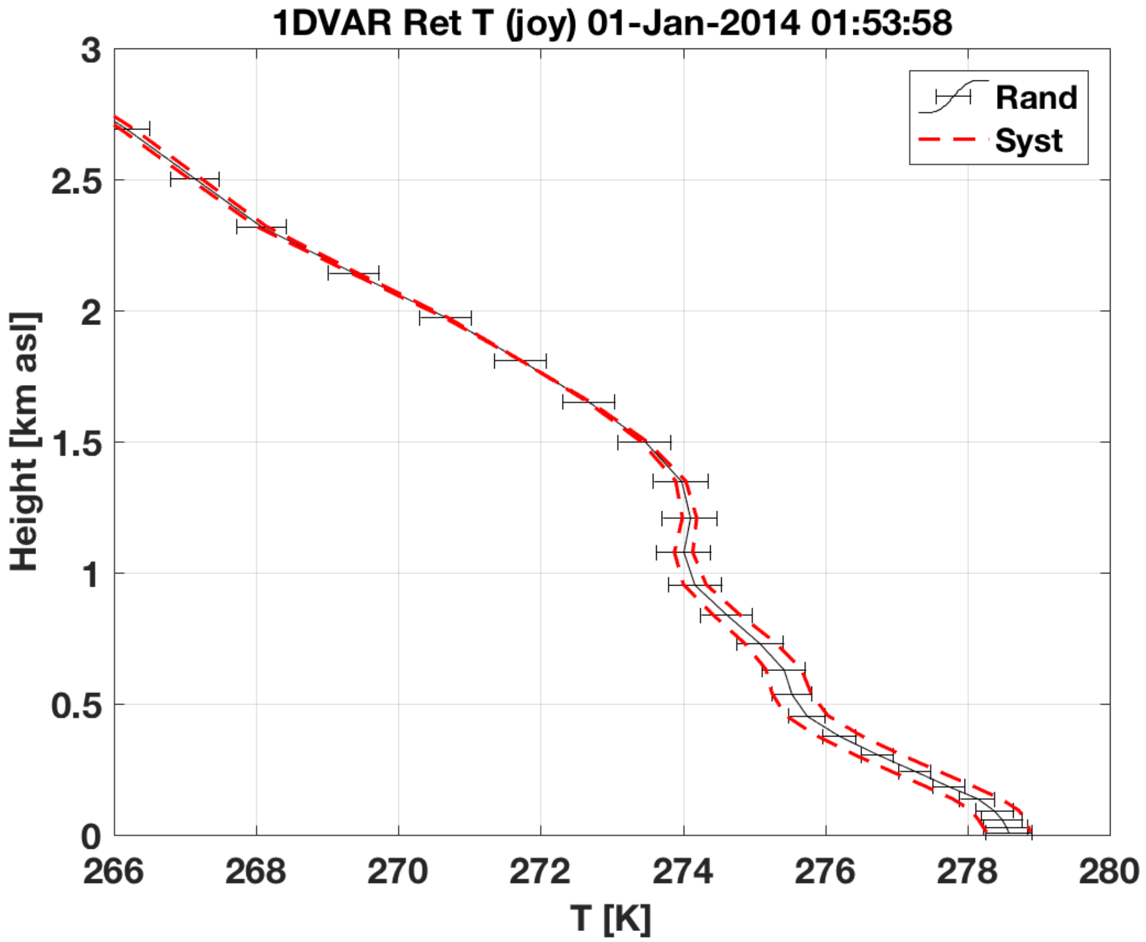

Figure 5. An example of temperature profile retrieval at the Joyce site (Juelich, Germany) on January 1st 2014, 01:53 UTC. The associated random (errorbars) and systematic (red dashed lines) uncertainties are also shown.

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.

References

Boukabara S. A., S. A. Clough, J.-L. Moncet, A. F. Krupnov, M. Yu. Tretyakov, and V. V. Parshin (2005), Uncertainties in the Temperature Dependence of the Line-Coupling Parameters of the Microwave Oxygen Band: Impact Study, IEEE Trans. Geosci. Rem. Sens., 43, 5, doi: 10.1109/TGRS.2004.839654.

Cimini, D., T. J. Hewison, L. Martin (2006), Comparison of brightness temperatures observed from ground-based microwave radiometers during TUC, Meteorologische Zeitschrift, Vol.15, No.1, 2006, pp.19-25.

Cimini, D., T. J. Hewison, L. Martin, J. Güldner, C. Gaffard and F. S. Marzano (2006), Temperature and humidity profile retrievals from ground-based microwave radiometers during TUC, Met. Zeitschrift, Vol. 15, No. 1, 45-56.

Cimini D., E. R. Westwater, and A. J. Gasiewski (2010), Temperature and humidity profiling in the Arctic using millimeter-wave radiometry and 1DVAR, IEEE Transactions on Geoscience and Remote Sensing, Vol. 48, 3, 1381-1388, 10.1109/TGRS.2009.2030500.

Cimini D. (2017), Report on G2.14: Missing uncertainty associated with MW absorption models, GAIA-CLIM 2nd General Assembly, ECMWF, Reading, Feb. 8-9, 2017.

De Angelis, F., Cimini, D., Hocking, J., Martinet, P., and Kneifel, S. (2016), RTTOV-gb – adapting the fast radiative transfer model RTTOV for the assimilation of ground-based microwave radiometer observations, Geosci. Model Dev., 9, 2721-2739, doi:10.5194/gmd-9-2721-2016, Online: http://www.geosci-model-dev.net/9/2721/2016/

De Angelis, F., Cimini, D., Löhnert, U., Caumont, O., Haefele, A., Pospichal, B., Martinet, P., Navas-Guzmán, F., Klein-Baltink, H., Dupont, J.-C., and Hocking, J. (2017), Long term Observations minus Background monitoring of ground-based microwave radiometer network. Part 1: Brightness Temperatures, Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2017-112, in review.

GAIA-CLIM Product Traceability and Uncertainty (PTU) document for the Microwave Radiometer (MWR) brightness temperature product (2017), PTU_MWR_Brightness_Temperature_V1.0.pdf

Hewison T. (2006), Profiling Temperature and Humidity by Ground-based Microwave Radiometers, PhD Thesis, Department of Meteorology, University of Reading.

Löhnert, U. and Maier, O. (2012), Operational profiling of temperature using ground-based microwave radiometry at Payerne: prospects and challenges, Atmos. Meas. Tech., 5, 1121-1134, doi:10.5194/amt-5-1121-2012.

Martinet, P., Dabas, A., Donier, J. M., Douffet, T., Garrouste, O., and Guillot, R. (2015), 1D-Var temperature retrievals from microwave radiometer and convective scale model, Tellus A, 67, 2015. Doi: 10.3402/tellusa.v67.27925.

Martinet, P., Cimini, D., De Angelis, F., Canut, G., Unger, V., Guillot, R., Tzanos, D., and Paci, A.: Combining ground-based microwave radiometer and the AROME convective scale model through 1DVAR retrievals in complex terrain: an Alpine Valley case study, Atmos. Meas. Tech. Discuss., https://doi.org/10.5194/amt-2017-144, in review, 2017.

Rodgers, C. D.: Inverse methods for atmospheric sounding: theory and practice, vol. 2, World scientific, 2000.

Solheim F., J. Godwin, E. Westwater, Y. Han, S. Keihm, K. Marsh, R. Ware (1998), Radiometric Profiling of Temperature, Water Vapor, and Liquid Water using Various Inversion Methods, Radio Science, 33, pp. 393-404, DOI: 10.1029/97RS03656.

Stähli, O., Murk, A., Kämpfer, N., Mätzler, C., and Eriksson, P. (2013), Microwave radiometer to retrieve temperature profiles from the surface to the stratopause, Atmos. Meas. Tech., 6, 2477-2494, doi:10.5194/amt-6-2477-2013.

Westwater E.R., S. Crewell, C. Mätzler: A Review of Surface-Based Microwave and Millimeter Wave Radiometric Remote Sensing of the Troposphere, URSI Radio Science Bulletin, No. 310, 59-80, 2004. Online: https://pdfs.semanticscholar.org/09ae/6c38f5d28fdd6c62703327c01a36d0d8af16.pdf

Westwater E. R., S. Crewell, C. Mätzler, D. Cimini: Principles of surface-based microwave and millimeter wave radiometric remote sensing of the troposphere Quaderni della Società Italiana di Elettromagnetismo Vol.: 1, No.3, 50-90, 2005. Online: http://radiometrics.com/data/uploads/2012/12/Westwater_QSIE_2005.pdf