

GAIA-CLIM



Work Package 2

Measurement uncertainty quantification

Karin Kreher (BKS) & the WP2 team











GAIA-CLIM GA, ECMWF, Reading (UK), 6-7 February 2017



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 640276.

Agenda

15:15-16:15 *Work Package 2. Measurement uncertainty quantification (Karin Kreher)*

15:15-15:30 Summary of the progress made to date in the 5 subtask 2.1.1 – 2.1.6, Karin Kreher, BKS

15:30 -15:45 Progress report on the development of best practices (task 2.3), Paul Green, NPL

15:45-16:00 Summary of the uncertainty assessment for the measurement capabilities provided to WP5 and discussion of the uncertainty questionnaires, Karin Kreher, BKS

16:00-16:15 Progress report on the uncertainty estimates identified for baseline network capability (task 2.2), Karin Kreher, BKS





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WP2 – Measurement Uncertainty Quantifications

Task 2.1 consists of six sub-tasks which are each instrument/ECV specific. In each case the aim is to either attain **metrologically traceable measurements** or achieve **substantial progress** towards this goal, plus to undertake a **detailed uncertainty quantification.**

- Production of traceability chains (building upon the QA4ECV project approach) plus numbers behind the boxes – every step needs a robust & quantitative assessment
- Documentation as to how to make the measurements, process the data and quantify the uncertainties (for each product to be included into the VO)
- Peer-reviewed publications

Task 2.2 identifying a defensible set of uncertainty estimates for a subset of ECVs with baseline network capability as identified by WP1.

Task 2.3 Review of the methodologies and tools for uncertainty quantification created under tasks 2.1 and 2.2 to ensure that the uncertainty traceability and measurement techniques follow best practice





 \rightarrow Guide to Uncertainty in Measurement & its Nomenclature

Task 2.1 – Development of reference quality measurement capabilities and uncertainty quantification

Structured in 6 "instrument" subtasks based on different measurement techniques (Lidar, MWR, FTIR, UV-Vis, MAX-DOAS, GNSS)

Main activities over the last 12 month:

- 1. Review of the GAID
- 2. Improvement of the uncertainty quantification and traceability chains (in close collaboration with NPL, Task 2.3)
- 3. Contribution to the VO (WP5) via the ROR table and D2.3





GAIA-CLIM WP2, task 2.1, 1. Review of GAID

- 1. GAID the existing gaps have been reviewed with focus on including any new information gained through assembling the traceability chains.
- 2. One FTIR gap has been retired and 2 new FTIR gaps have been identified by the TCCON community:

(A) Lack of FTIR sites with high/low albedo and Carbon emissions hot spot monitoring

TCCON sites located in regions with high or low albedo are missing. Since retrievals could be biased by the albedo, observations at such sites would help investigating the existing biases in the satellite retrievals.

(B) In addition a possible gap relating to "**Higher and faster measurement frequency by automatic measurement and retrieval for FTIR**" was identified and will be included in the next version of the GAID.

3. During last couple of weeks: All existing gaps have been reformatted into the new template, still ongoing for some of the gaps.
Another round of reviews would be helpful.





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Task 2.1.2: Temperature and H₂O profiles measured by microwave radiometers

Technical: NIST

Knowledge:

Governance:

TOPROF

GAIA-CLIM

- Contribute to the GAID (5 entries)
 - G2.13: Missing MW standards maintained by Metrological Institute
 - G2.14: Missing the uncertainty associated with MW absorption models used in MWR retrievals
 - G2.15: Lack of unified tools for automated MWR data quality control
 - G2.16: Missing agreement on calibration best practices and instrument error characterization
 - G2.17: Lack of a common effort in homogenization of retrieval methods

GAIA-CLIM WP2, task 2.1, 2. Uncertainty quantification and traceability chains

Specific updates to the previously presented chains:

1) Traceability chain for total column ozone measured with UV-visible spectroscopy (shown in the next slide)

- 2) Developments to make the traceability chains more valuable and more attractive to use for the user: e.g. interactive traceability chain boxes which bring up background information when clicked (examples can be downloaded from the GAIA-CLIM webpage).
- 3) GAIA-CLIM traceability chains and uncertainty quantification study for ozone observations presented at the QOS 2016 in Edinburgh in September, showcasing the traceability chain and processing steps for LIDAR, FTIR and UV-visible spectroscopy
- 4) No traceability chain yet developed for tropospheric ozone measured by MAX-DOAS but an extensive intercomparison campaign (CINDI-2) was held in the Netherlands in September including more than 30 MAX-DOAS instruments from 24 different groups. The results are expected to provide valuable background



material for further development in processing procedures and uncertainty quantification.



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Aerosol extinction coefficient (Raman method)



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WP 2, Task 2.1.3

- Presentation at ACVE Oct 2016
- Presentation at IRWG on GAIACLIM and QA4ECV CO harmonisation
- Uncertainty harmonisation required updating retrieval scripts: shared between GAIACLIM and QA4ECV
- Now working on GAIACLIM NDACC FTIR targets: CH4 and O₃









GAIA-CLIM WP2, task 2.1, 2. Uncertainty quantification and traceability chains

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Second <u>Cabauw Intercomparison of Nitrogen Dioxide measuring Instruments</u>

CINDI-2 data products: Ozone, NO₂, Formaldehyde, O₄, aerosol

CINDI-2 Semi-blind Intercomparison 12 - 28 September 2016 Cabauw, The Netherlands







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What do we want to achieve with CINDI-2 in comparison to CINDI

- > To follow on from previous intercomparisons by Roscoe et al. (1999), Vandaele et al. (2005) and <u>Roscoe et al. (2010)</u> and to apply recommendations made:
 - synchronisation of measurements (very detailed measurement protocol)
 - exact alignment of the elevation angle (horizon scans & lamp measurements)
 - more groups (24) & more instruments (33)
 - more viewing directions (7 for 2d instruments)
 - profiling techniques

Semi-blind intercomparison protocol (NDACC)

- Measurement from the previous day have to be provided to the campaign referee by 10 am.
- At a daily meeting (4 pm), slant columns measured during the previous day were displayed without assignment to the different instruments.
- The referee notifies instrument representatives if there is an obvious error so that this can be corrected for the rest of the campaign.
- At the end of the formal campaign, plots have instrument names attached, and plots of mean differences from one selected reference instrument or an average of several selected reference instruments are discussed.
- After the end of the formal campaign time, revisions are only accepted where full details of the reasons for changes are supplied.





Diagnostics for discussions during the daily meetings

- Daily time series for most of the species (2xNO2, 2xO4, 2xO3, HCHO)
- Relative differences (daily and longer time period)
- Correlation plots
- Plots with summary of regression analysis from correlation plots







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Elevation= 5°, 0°<SZA<100°, All azimuths





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	NO2vis		NO2visSmall		NO2uv		O4vis			O4uv		НСНО		O3uv			O3vis							
	slope	offset	RMS	slope	offset	RMS	slope	offset	RMS	slope	offset	RMS	slope	offset	RMS	slope	offset	RMS	slope	offset	RMS	slope	offset	RMS
bira4	1.02	-0.61	4.79	1.03	-0.52	4.46	1.02	0.43	3.09	1	0.3	1.58	1.01	0	0.74	0.97	7.25	5.01	1.01	0	0.13	1.01	0.46	0.57
auth3				0.96	1.03	5.45	1.01	-2.07	6.25				1.04	-0.71	2.69	1.17	2.68	18	1.01	0.01	0.23			
aiofm1		-	-				0.81	3.83	28.58				0.93	-0.17	2.37	0.82	13.55	19.12	1.67	-0.1	3.48			
iuph19		-		0.95	0.57	4.76	0.98	0.09	12.54				0.95	0.91	1.89	0.94	-2.47	15.05	0.96	-0.02	0.26	1.07	3.4	3.87
iupb18	1	0.74	4.15	1.02	0.51	3.76	1.02	0.83	2.74	0.99	0.33	1.38	0.96	0.85	1.39	1.06	3.08	5.2	1	0.01	0.35	1.01	0.05	0.33
boku6	1.04	0.71	5.61							1	0.63	1.74			1							1.02	-0.36	0.63
cma7				0.96	2.09	10.6	0.96	1.87	7.34				1.03	-0.63	2.07	0.81	1.1	12.73	0.95	-0.04	0.29			
cma8	0.99	-0.76	4.2							1	0.14	3.17										1.11	9.3	23.08
chiba_u9	0.92	0.09	5.46	0.94	-1.32	5.31	0.92	-0.23	3.66	0.94	2.97	2.8	0.93	1.56	1.14	0.8	8.33	8.15	0.82	0.08	0.15			
csic10							0.83	-8.56	26.45				0.89	-8.09	23.48	1.22	-29.91	59.66	0.83	-0.32	2.36			
cu-boulder11				0.73	10.3	17.07	1.00	-3.20	9.04				1.03	-1.35	2.29	1.01	-3.26	10.39				0.99	-0.58	0.89
cu-boulder12				0.99	-3.18	18.18	0.99	-3.04	12.34				0.87	1.79	7.13	0.33	27.27	23.89	0.88	0.35	1.38			
dlrustc13	0.94	1.99	5.53	0.96	1.13	4.38	0.97	-0.29	2.98	0.95	0.47	2.12	1.01	-0.02	1.14	1.09	-6.81	6.6	1	0.66	0.74	1.03	0.84	1.01
dlrustc14	0.98	1.46	4.31	1	1.16	3.64	1.01	0.31	2.38	0.97	0.47	1.57	1.01	0.33	0.87	1.23	-12.38	9.24	0.98	0.7	0.72	0.97	-0.46	0.61
iiserm16				1.06	-0.18	5.26	1.02	0.97	4.80				1.07	0.7	1.81	0.77	-20.06	20.51	0.81	-0.04	0.31			
inta17	0.97	0.44	3.93							0.99	0.25	2.07										1	0.48	0.81
knmi21							0.98	-2.18	3.62				1.02	0.32	1.43	0.84	-7.48	15.01						
knmi22	0.91	1.46	8.2							0.98	0.4	2.67												
knmi23	1.03	-3.51	14.47	1.03	-0.86	10.92	1.01	-1.18	40.30	1.11	-9.29	15.4	1.04	-1.1	12.53	1.02	-2.79	23.04	1.04	-0.11	1.64	1.03	-2.32	10.6
luftblick26	0.96	3.37	6.82	1.03	-6.39	11.93	1.01	-0.30	2.77	0.99	4.39	13.12	1.02	-0.49	1.32	1.06	-2.95	11.14	1.01	0.02	0.23	1	2.16	7.42
luftblick260	1.05	-4.92	10.28	0.97	9.48	12.84				1.05	-6.29	13										1.06	-3.99	9.09
luftblick27	0.99	-0.24	2.33	1	-0.43	2.03	0.99	0.09	2.63	1.01	-0.19	1.03	1	-0.3	1.15	1.01	-0.58	9.48	0.98	-0.01	0.19	0.98	-0.19	0.36
luftblick270	0.99	-0.4	2.22	1.01	-0.07	2.08				1	-0.17	0.9										1	0.53	0.51
mpic28				1.01	2.04	5.91	1.03	1.78	4.01				1.02	-0.07	0.92	0.93	6.67	5.04	1.02	0.01	0.15			
nasa31	1	1.48	15.24	1	1.11	13.99	1.01	0.86	10.35	0.98	0.34	5.14	0.96	0.4	5.52	0.94	-3.01	22.37	1.01	-0.02	0.48	0.98	0.01	2.13
nasa32	0.98	3.27	7.31	1.02	-2.91	8.24	1.01	-0.13	5.10	0.95	4.65	10	1.02	0.33	3.12	1.08	-6.07	17.98	1	0.05	0.35	0.98	1.09	6.08
niwa29	0.98	-0.68	3.58	0.99	-0.73	2.98	1.01	-0.09	1.95	0.96	-0.98	2.4	0.98	0.92	1.03	0.75	5.63	7.09	1	-0.01	0.1	1.04	-1.55	1.46
niwa30	0.95	0.38	3.46				0.87	3.02	7.54	0.97	0.13	1.7	0.93	-0.05	2.68	0.99	-0.52	6.85						
nust33				0.88	-0.17	13.38	0.91	-0.72	12.50				0.76	-0.42	3.61	1.73	-8.97	38.22						
Imumim35	1.06	0.58	11.33	0.91	2.82	8.41	0.91	0.79	5.52	1.02	1.36	3.78	0.94	0.87	1.71	0.82	-3.81	8.2	0.82	-0.25	1.37	1.04	-1.79	5.21
uto36	0.92	-0.16	4.98	0.94	0.24	4.38				0.96	-0.16	1.68										0.93	-0.41	0.83
amoiap2	0.92	-0.13	3.33	0.91	0.34	2.91	0.97	-0.96	4.56	1.06	-2.48	3.69	0.93	-1.01	2.13	1.04	-10.71	14.66						
latmos24																								
latmos25																								
bsu5							0.92	0.88	4.08				0.99	-1.37	0.9	0.96	15.66	20.53	0.88	-0.19	0.3			
P10	0.94	-2.18	2.93	0.94	-3.21	2.83	0.93	-2.41	2.64	0.95	-3.77	1.24	0.93	-1.12	0.9	0.78	-12.62	5.34	0.9	-0.34	0.14	0.95	-2.51	0.42
P25	0.97	-0.96	3.84	0.97	-0.88	4.07	0.95	-0.91	3.09	0.98	-0.34	1.65	0.95	-0.67	1.14	0.88	-6.22	8.15	0.93	-0.04	0.22	0.97	-0.66	0.62
Median	1	0	4.98	1	0	5.38	1.00	0.00	4.95	1	0	2.4	1	0	1.85	1	0	13.69	1	0	0.31	1	0	1.01
P75	1.03	0.96	7.54	1.03	0.88	11.43	1.05	0.91	10.35	1.02	0.34	4.12	1.05	0.67	2.69	1.12	6.22	20.51	1.07	0.04	0.9	1.03	0.66	5.86
P90	1.06	2.18	12.59	1.06	3.21	14.3	1.07	2.41	25.06	1.05	3.77	13.05	1.07	1.12	6.97	1.22	12.62	23.8	1.1	0.34	1.93	1.05	2.51	9.99





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GAIA-CLIM WP2, task 2.1, 3. Contribution to the VO (WP5) via the ROR table

 ROR (Reference Observations Readiness) table entries developed together with WP5 and WP3;

internal tool to help us coordinate our efforts between WP2, WP3 and WP5 for data product input into the VO.

- This activity was followed by an Uncertainty assessment for the measurement capabilities provided to WP5 (D2.3)
- **Aim:** To provide the necessary information to allow the development of user support tools by the WP5 VO team.





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Task	Technique	ECV	Tracea- bility chains	Uncertainty budget behind the chain steps	Available literature	GAIA-CLIM documen- tation		
T 2.1.1	Lidar	Aerosol, T, O3, H2O	\checkmark					
T 2.1.2	MWR	H2O, T	\checkmark					
Т 2.1.3	FTIR	CH4, CO2, H2O, O3	✓					
T 2.1.4	UV-Vis	03	\checkmark					
Т 2.1.5	MAX- DOAS	Trop. O3	X					
T 2.1.6	GNSS	H2O	\checkmark					





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Overview Table, also for task 2.1 meeting on Thursday

Questions?





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GAIA-Clim related work of the project MUSICA (2011-2016)





Network-wide consistency documentation by using atmospheric CO₂ as standard metric:



Aerosol extinction coefficient (Raman method)

Calibration: The processing requires the assumption of:

1) Molecular profiles of backscattering coefficient at Raman wavelength λ_R , and of extinction coefficients at laser and Raman wavelengths λ_L and λ_R . These profiles are calculated from models of molecular scattering cross section and a molecular number density profile, retrieved from Standard Atmosphere, radiosondes or mesoscale models;

2)Angstrom exponent, describing the wavelength dependence of aerosol extinction coefficients at wavelengths λ_L , and λ_R . Fixed values (0 for cirrus clouds and 1, 1.5 or user-defined values, variable according to actual meteorological conditions) are usually used. Alternatively, values measured with sun photometers or derived from multi-wavelength simultaneous measurements of extinction coefficient are used.

Vertical smoothing: The processing requires the calculation of the derivative of the logarithm of the preprocessed Raman signals. There are several methods to calculate derivative. the The most common methods use linear fit or digital filters, such as Savitzky-Golay filter. The calculation of the derivative implies a vertical smoothing of aerosol extinction coefficient profile and а reduction of its vertical resolution and statistical uncertainty with respect to the pre-processed Raman signals.

Standard uncertainty: The standard uncertainty of aerosol extinction coefficient profile can be estimated with the Monte Carlo method or analytically, by means of error propagation theory.

Standard uncertainty

Multiple scattering correction: the profile of aerosol extinction coefficient can be corrected for multiple scattering. This affects the extinction coefficient retrieval in an optically dense medium, as fog and clouds. When the laser beam goes through this medium, not only the singly backscattered photons, but also photons undergoing multiple scattering processes remain in the lidar receiver field of view and are forwarded to the receiving system. In these conditions, lidar equations and algorithms, valid only in single scattering approximation, lose their validity. The multiple scattering makes lidar signals higher and extinction coefficient lower than those measured in single scattering conditions. The correction is performed by introducing in lidar equations correction factors, estimated from multiple scattering models (e.g. Eloranta, 1998). These calculate multiple scattering intensities for lidar returns, considering the properties of the scattering medium and of the lidar system.



Aerosol extinction coefficient (Raman method)





- Rigel Kivi: ongoing work on new Aircore measurements
- Matthias Schneider: ongoing work in MUSICA, uncertainty harmonisation







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Task 2.1.6: Total Column Water Vapour measured by GNSS

K. Rannat (TUT), J. Jones (MO)

Aim: Analyse the **uncertainties for total column water vapour** measured by GNSS and **improve traceability** of the GNSS measurements.









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Software-dependent differences in GNSS-PW uncertainty budget

Practical experiments with "as close as possible" experimental set-ups for different software with identical observational information.

Doing what:

Processing GNSS-data (next slide), obtaining ZTD (and ZTD uncertainties), deriving GNSS-PW, calculating GNSS-PW uncertainties according to T.Ning etal 2016, analysing the differences and the main factors introducing these differences.

Later comparing with PPP-solution from GIPSY.

Choosing COST BENCHMARK sites (ref. Slide 4) – allows to compare with results obtained from independent ACs involved in COST-action.

Some software development (TUT):

Tools for extracting site meteodata from MO-meteodata format \rightarrow site metRINEX (for GAMIT) Tools for ZTD \rightarrow IPW + GRUAN-like uncertainties

Tools for driving experiments with GIPSY and comparing/analysing the results





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GNSS IPW: The same Metrological Model Chain with different software ?



Experimental sites from COST BENCHMARK campaign





«Yellow» – GNSS-sites «Green» – co-located meteorological stations



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