GAIA-CLIM deliverable D1.2

Gap Analysis for Integrated Atmospheric ECV CLImate Monitoring:

Modelling studies of the impacts of gaps – experimental design

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1. Summary

This report defines and describes the model simulations used as part of GAIA-CLIM Task 1.5. Background is given in Section 2. The definition of the model simulation is presented in Section 3, grouped along the topics to be addressed and the corresponding models. Greenhouse gas observations of CO_2 and CH_4 are addressed with the TM3 model by MPI BGC. BIRA is addressing the issue of air quality and short lived climate forcing gases, in particular carbon monoxide, CO, through inverse modeling with the IMAGESv2 model system. Aerosols are addressed with aerosol climate modeling using the ECHAM-HAMMOZ model by FMI. Ozone and related trace gases are addressed through chemistry climate modeling using the EMAC model system by KIT. This is briefly summarized in Table 1.

2. Background

The model based assessment of gaps in observing system capabilities complements and extends the activities within GAIA-CLIM by addressing the questions like (according to the GAIA-CLIM Description of Action):

- Where the in-situ capabilities are noted to have gaps, or to lack a transfer standard, then do these need to be filled by additional in-situ data, or is a model-based interpolation or analysis based field estimate a plausible alternative means of EO sensor characterisation?
- Where, based upon our understanding of atmospheric processes, would additional measurements add most interpretative value to EO sensor characterisation?
- Does measurement frequency, scheduling or quality matter more? What would be the trade off between these in terms of our ability to characterise EO sensor performance?
- Do fewer measurements in fewer locations with lower uncertainties have benefits over more measurements at more locations but with higher uncertainties?

Within the planned work of Task 1.5 there is a clear emphasis on the first two questions. Ultimately, progress in Task 1.5 may enable us to address also the last two questions, but this is less clear at present.

The GAIA-CLIM Gap Assessment and Impacts Document (GAID) has categorized known gaps into seven generic gap types:

1. coverage (spatiotemporal)
2. vertical resolution (profile, per troposphere/stratosphere altitude domain)
3. uncertainty (per observation, unc. budget, calibration)
4. uncertainty (in relation to comparator measures, representativeness)
5. technical (formats, conventions etc)
6. governance (harmonisation procedures, 24/7, etc)
7. parameter (need for auxiliary information/parameters).

In order to meet these goals, a number of modeling groups, each representing expertise in a key area relevant for GAIA-CLIM, have been incorporated. The groups involved and model systems used have been selected to cover a wide range of topics, including experts in greenhouse gas modeling, air quality and inversion modeling, aerosol modeling and chemistry climate modeling. Each of the groups is actively involved in further international modeling activities (e.g., such as the WCRP-SPARC / IGAC Chemistry Climate Modelling Initiative, CCMI).

Max Planck Institute for Biogeochemistry contributes with their expertise in modeling of greenhouse gases (CO_2 and CH_4) and inverse modeling. Likewise, BIRA contribute with modeling of air quality and short lived climate forcing gases (in particular CO) and inverse modeling of their sources and sinks, such as investigation of the hydroxyl radical (OH) as a sink for CO. FMI contribute with aerosol climate modeling and KIT with chemistry climate modeling to address the climate impact on ozone and related trace gases. KNMI and ECMWF do not contribute with own model runs, but provide input to this Task. A specific (in kind) KNMI contribution to this WP is to pass through the latest relevant information on validation results from MACC/CAMS which are documented in 3-monthly MACC/CAMS validation reports published here http://atmosphere.copernicus.eu/validation.

In terms of the gap type characterization, most of the modeling work within this task addresses gaps in coverage and representativeness, as well as gaps in available parameters, e.g. with respect to multivariate dependencies.

3. Definition of model simulations and planned analyses

In this section, the model simulations to be performed or used are described, together with an outline of the specific analyses to be performed. The presentation is organized along the topics to be addressed, together with the specific model systems to be used: (1) Greenhouse gases CO_2 and CH_4, (2) air quality and short lived climate forcing gases (CO), (3) aerosols and (4) ozone and related trace gases. Table 1 summarizes the topics addressed and models involved.

Table 1: Topics addressed in WP 1.5 by specific models, the respective ground-based observational networks addressed, and the institutions responsible for this part of the work.

	Model	*Technique*	*Network addressed*	*Institution*
Greenhouse gases, CO_2 and CH_4	**TM3**	**Global tracer transport model**	**TCCON**	**MPI BGC**
Air quality, CO	**IMAGESv2**	**Inverse modelling**	**TCCON**	**BIRA**
Aerosols	**ECHAM-HAMMOZ**	**Aerosol Climate model**	**AERONET**	**FMI**
Ozone and related trace gases	**EMAC (ECHAM5-MESSy2)**	**Chemistry Climate model**	**NDACC**	**KIT**

3.1 Greenhouse gases, CO_2 and CH_4 (MPI BGC)

This work focuses on the model-based analysis of the atmospheric greenhouse gases CO_2 and CH_4. Here the main validation network currently available consists of the FTIR sites of TCCON, and this study first aims to describe how well the variability in the atmosphere is sampled by TCCON. That is, over what spatiotemporal domain the current measurement capabilities can be considered to well characterize the volume mixing ratios in the atmosphere.

We will assess the variability and correlation of atmospheric total-column CO_2 and CH_4 in order to identify regions of high variability nearby TCCON sites on different time scales (focussing on synoptic and seasonal). The aim is to determine the “area of influence” of the FTIR column measurements, within which the spatial variability of these tracers can be ignored with respect to the current capabilities of satellite instruments. In other words, we assess the representativeness of each FTIR site and their potential spatial and temporal applicability in validating satellite observations.

In addition to this approach, a parameter-based gap assessment will be carried out. At present most XCO_2 and XCH_4 retrievals employ bias corrections which are based on multivariate dependencies on various geophysical quantities, such as surface albedos at different wavelengths or retrieved aerosol optical depth. An additional parameter-based analysis is planned to assess how well the satellite measurements that are co-located with TCCON sites currently sample this parameter space.

3.1.1 Scope of the assessment

This analysis aims to address primarily the first two questions raised in section 2. Specifically, the gaps of the measurements in space and time (gap type 1) are assessed while using an atmospheric model to extend the domain over which the measurements can be considered to be representative, taking into account the measurement uncertainty to define the matching threshold (assessing gap type 4). These gaps are again assessed based on the transport- and flux-influenced colocation criteria determined by the model simulations, but this time in parameter space, considering geophysical parameters that are believed to influence systematic errors in satellite retrievals. Here gap type 7 is characterized to answer the first question.

Based on these descriptions of gaps, the second question can be addressed, indicating where additional stations could optimally extend the network both in terms of geographical and in terms of geophysical parameter space.

3.1.2 Model used

We will be utilizing forward simulations generated by the global tracer transport model TM3 (Heimann and Körner, 2003) at the highest available global spatial resolution (1.125 ° x 1.125°).

3.1.3 Simulations that will be run

The additional forward simulations required for this work are minimal, with one simulation for CO2 and one for CH4, encompassing one year plus spin-up. They are based on flux maps already available. It is planned to use the year 2010, as it is one of the two full years (with 2011) with both GOSAT and SCIAMACHY measurements available.

3.1.4 Additional data needed

The location and sampling of the TCCON sites are necessary input for this study. The latest version of TCCON data is readily available at http://tccon.ornl.gov. For the parameter analysis it is necessary to use the auxiliary data from relevant satellite measurements as well as additional data available from the XCO_2 and XCH_4 retrievals. These parameters include albedos at different wavelengths, solar zenith angle, retrieved aerosol parameters, etc. These parameters are available in the L2 data files from both GOSAT and SCIAMACHY, which are already on hand.

3.1.5 Planned analysis

Using the set of column-integrated volume mixing ratios simulated by TM3 model we will generate spatial plots of the area of representativeness of each site for validating satellite measurements. We will take into account random errors of the satellite observations and use appropriate co-location criteria, based on the convolution of transport and flux variability. The approach is based on the colocation criteria used for GOSAT-TCCON validation proposed by Guerlet et al. (2013).

For the parameter-based study, the multivariate space covered by all the satellite soundings for one year will be mapped. The subset of these satellite soundings which are collocated with TCCON measurements will be defined, again based on the match criteria of Guerlet et al. (2013). This subset of soundings will be mapped into the multivariate parameter space, allowing for the identification of regions of this space currently under-sampled by TCCON.

These analyses will allow for the identification of locations where additional column measurements would most benefit the validation of spaceborne XCO_2 and XCH_4 observations, based on gap types 1, 4, and 7.

3.2 Air quality, carbon monoxide (BIRA)

3.2.1 Scope of the assessment

The objective of BIRA will be to determine whether the current network of vertically resolved FTIR data for carbon monoxide is sufficient to provide (in combination with EO data) helpful additional constraints on the budget (sources *and* sinks) of this compound. In several previous modelling studies, ground-based measurements (CMDL, now GMD) and/or satellite data (MOPITT, AIRS, IASI,…) have been used in conjunction with global CTMs to provide top-down constraints on the surface emissions and (in some cases) also the photochemical production of CO. In such studies, a set of emission parameters (with their specified error covariances) are varied in a CTM in order to reproduce a given set of atmospheric measurements to within their uncertainties. Unfortunately, the resulting optimized emissions prove to be sensitive not only to the choice of atmospheric dataset (e.g. ground-based vs. satellite) and inversion setup (e.g. number of emission parameters, assignment of errors on emissions and on the measurement data, choice of either fixed or variable photochemical production due to hydrocarbon oxidation) but they are also greatly influenced by the representation of the chemical sink of CO, i.e. the abundance of hydroxyl radicals (OH). For example, as average OH levels are likely overestimated by most models in the Northern Hemisphere according to analyses of methyl chloroform (MCF) observations, for reasons still unclear, the total hemispheric top-down CO emissions are likely too high. To address this issue, we will 1) use the (low resolution) MCF-derived constraints on OH fields in source inversions, and 2) use vertical CO profile measurements by ground-based FTIR instruments from the TCCON network as additional constraints in the source optimizations, since vertical concentration gradients reflect the effects of chemical sinks. Vertical FTIR data are scarce, but better characterized than vertical information from satellites. The latter could however be used in a next step.

3.2.2 Model used and planned simulations

The model to be used is IMAGESv2 (Stavrakou et al., 2015) in an inverse modelling framework based on its full adjoint model (Müller et al., 2005; Stavrakou and Müller, 2006). This model will be run for the year 2010 at 2°x2.5° horizontal resolution with 40 vertical hybrid levels, using ECMWF ERA-Interim meteorology. Emission inventories will include GFEDv3 emissions for biomass burning, MEGAN-MOHYCAN for biogenic NMVOCs, EDGARv4 and a blend of regional inventories for anthropogenic compounds. The chemical mechanism is comprehensive, with > 120 compounds and a detailed mechanism in particular for isoprene.

3.2.3 Planned analysis

The following steps are foreseen:

S1. Regular inversion of CO sources, using methodology similar to Stavrakou and Müller (2006), based on surface concentration measurements (GMD) and *total* columns by ground-based FTIR stations and satellite (IASI) CO measurements, in order to generate a best model estimate of OH concentrations, $[OH]_{mod}$ (4-d distribution, month x latitude x longitude x vertical level). The inversion involves the minimization of a cost function which quantifies the overall bias between model and observations, and includes a regularization term penalizing the solutions too different from the a priori.

S2. Modify $[OH]_{mod}$ to match constraints from MCF (crude scaling by latitude bands) →best estimate $[OH]_{best}$ but also interval from $[OH]_{min}$ and $[OH]_{max}$ based on the uncertainties on the constraint

S3. Perform series of source inversions based on ground-based GMD data and CO total columns from FTIR stations and IASI, using different [OH] fields obtained from previous step. [OH] will be varied separately in different large latitude bands.

S4. Analysis of the different inversions in previous step, focusing on their performance against (not only GMD and IASI data but also) vertical profiles at FTIR CO stations. Determination of the best set of emissions and OH fields – although the differences between different solutions might be small in comparison with uncertainties related to other parameters. Sensitivity studies exploring the effect of, for example, alternative a priori emissions, emission set-ups, or vertical mixing parameterizations will be conducted to assess these effects.

S5. If time allows, the steps S3-S4 above might be (partly) repeated using alternative chemical datasets (e.g. including vertical CO profiles) as constraints to the inversion.

The model simulations and analysis will be performed in 2016. The main output of this part of the study will be

(1) an updated top-down determination of CO emissions and photochemical production, including an assessment of their sensitivity to errors in [OH] as well as other model parameters

(2) a determination of the added value of vertically resolved CO data at FTIR stations

3.3 Aerosols (FMI)

For atmospheric aerosols, FMI will investigate observational gaps with respect to representativeness of in-situ data as well as additional data needs. The studied ECV is aerosol optical depth (AOD), but also other optical properties (such as single scattering albedo, Ångström exponent and absorption optical depth) will be looked at. Given the short lifetime of atmospheric aerosols (from hours to ~1 week in the troposphere) and the relatively sparse temporal resolution of satellite-based observations (pass over a specific site every 0.5-16 days depending on the instrument), it is likely that satellites miss out on some aspects of the atmospheric aerosol variability. Further limitations of most satellite instruments are that they can observe aerosols only in cloud-free conditions, there are no observations during nighttime, and information on composition in very limited. On the other hand, the surface-based Aerosol Robotic Network (AERONET) (Holben et al., 1998) provides long-term, continuous measurements of AOD and other aerosol optical and radiative properties from dozens of (mostly continental) measurements sites. These continuous measurements enable a good characterization of local aerosol variability; however reasonable geographical coverage is obtained only over parts of Europe and US, and elsewhere long-term AERONET measurements are very scarce. Given these respective limitations of both satellite and surface-based observations, it is important to identify the geographical regions that currently suffer from poor observational constraints of aerosol properties in order to guide the development of future observational capabilities. The work within GAIA-CLIM focuses on assessing the representativeness of the network in terms of aerosol temporal and spatial (both vertical and horizontal) variability.

3.3.1 Scope of the assessment

The analysis addresses primarily the first two questions raised in section 2. Similarly to section 3.1, the gaps of the measurements in space and time (gap type 1) are assessed by using an aerosol-climate model to extend the domain over which the measurements can be considered to be representative. Measurement uncertainty is taken into account to define the matching threshold (gap type 4). This analysis is utilized to address the second question outlined in section 2, i.e. where additional measurements would add most interpretative value to EO sensor characterisation.

3.3.2 Model used

The global aerosol-climate model used will be ECHAM-HAMMOZ (Stier et al., 2005; Zhang et al., 2012; Bergman et al., 2012) run with T63 vertical resolution.

3.3.3 Simulations that will be run

The work will require new simulations, which are however straightforward to perform. The baseline simulation will be a 10-year nudged run using the standard ECHAM-HAMMOZ set-up. In addition to calculating the traditional global aerosol 3-D fields (proxy for real atmosphere), we will also sample the model output online according to real satellite overpasses (proxy for what the satellite sees). The two different outputs will be compared to each other to identify in which regions the measures of aerosol variability may be biased in satellite observations. Both temporal and spatial (horizontal and vertical) variability will be investigated. The satellite-collocation sampling procedure in the model (JASMIN Community Intercomparison Suite; http://proj.badc.rl.ac.uk/cedaservices/wiki/JASMIN/CommunityIntercomparisonSuite) has already been implemented within ECHAM-HAMMOZ during previous projects. The traditional 3D-fields (proxy for real atmosphere) will be used also to investigate the representativeness of individual AERONET sites.

3.3.4 Additional data needed

Observational data from the AERONET network is freely available at http://aeronet.gsfc.nasa.gov/. The studied ECV is aerosol optical depth (AOD), but also other optical properties (such as single scattering albedo, Ångström exponent and absorption optical depth) will be investigated.

3.3.5 Planned analysis

In terms of representativeness of the measurement sites, the planned analysis is similar to the approach outlined in section 3.1.5. Based on this analysis, locations where new AERONET-type measurements would be most beneficial will be identified. It should be noted that the chosen approach relies on the assumption that the ECHAM-HAMMOZ model is capable of capturing the qualitative features of atmospheric aerosol variability, and thus can be used to identify gaps in current observation systems in terms of geographical coverage. To evaluate the validity of this assumption, we will perform a detailed comparison of the modelled and the observed aerosol variability at a selected subset of AERONET sites in different environments. The results from this comparison will be used to evaluate the validity of our gap analysis.

3.4 Ozone and related trace gases (KIT)

The evolution of the stratospheric ozone layer over the 21st century will be controlled by the decreasing concentration of ozone depleting substances (ODS) following the Montreal Protocol and its amendments as well as by climate change due to the increase of greenhouse gases. Tropospheric ozone, itself a greenhouse gas, will also be influenced by changes in precursor emissions and indirectly by climate change due to the increase of greenhouse gas concentrations. One sensitive region is the tropics, where chemistry climate models predict that stratospheric ozone will not recover by the reduction of ODS, but will further decrease due to changes in large scale circulation (enhancement of the Brewer-Dobson circulation) as a result of increased concentrations of greenhouse gases. A clear attribution of past changes in tropical column ozone however is complicated by uncertainties in concurred increases in tropospheric ozone (e.g., Shepherd et al., 2014). This is further complicated by the paucity of stable long-term sub-orbital ozone observations in the tropical regions.

3.4.1 Scope of the assessment

We will use simulations with the chemistry climate model EMAC to help characterizing the quality and ability of existing ground-based observational networks to retrieve climate change related signals in ozone. In particular we will investigate how the results will depend on the vertical resolution of the observations, the ability of the observations to separate tropospheric and stratospheric ozone contributions, as well as the geographical representativeness of the existing networks (e.g., addressing the existing bias in coverage between Northern and Southern Hemisphere in the existing networks, as expressed in the Gap Assessment and Impacts Document).

3.4.2 Model system and simulations used

The EMAC model system is based on the German climate model ECHAM in version 5 (Röckner et al., 2003) and the Modular Earth Submodel System (MESSy) in version 2 (Jöckel et al., 2006; Jöckel et al., 2010). We will base our analysis for the past decades on an EMAC simulation over the period 1979 – 2014 with comprehensive chemistry, nudged towards ECMWF ERA-Interim re-analyses, that has recently been completed at KIT. This simulation will be sampled at a number of network sites with high-temporal resolution (one hour). In addition, full 3D fields are available for further analyses with reduced temporal resolution (11 hours). The future simulation will be based on an EMAC simulation run over the period from 1960 – 2099 as part of the Earth System Integrated Modelling (ESCIMo) consortium (Jöckel et al., 2015). The future simulation follows REF-C2 specifications of the WMO-SPARC/IGACC Chemistry Climate Modelling Inititative (CCMI), using the Representative Concentration Pathway (RCP) 6.0 scenario for future greenhouse gas emissions. Both of the EMAC simulations are performed in T42 horizontal resolution, corresponding to 2.8°x2.8°, and 90 vertical levels from the ground up to the mesosphere. While we have some flexibility within this project to perform additional model simulations if deemed necessary further on in the project, a complete re-run of a climate change simulation over the 21st century is prohibitive due to the large computational cost: E.g., the recently completed REF-C2 simulation from 1960 – 2099 used more than 1 million CPU-hours and almost 1 year of wall-clock time (Jöckel et al., 2015). The availability of the two recently completed simulations for this project guarantees that all foreseen analyses within this task with respect to ozone and related trace gases can be performed.

3.4.3 Additional data needed

The analyses with respect to ozone and related trace gases will address primarily, although not exclusively, observations from the ground-based NDACC network. This work will benefit from the existing strong connections with the NDACC network (Task Leader B.-M. Sinnhuber (KIT) is a member of the NDACC Scientific Steering Committee).

3.4.4 Planned analysis

Model simulations over the past decades, nudged towards meteorological re-analyses from ECMWF ERA-Interim, will be provided at the location of existing long-term observations. We will investigate how the characterization of long-term changes will depend on vertical resolution (and in particular the ability to separate tropospheric and stratospheric contributions) by degrading the vertical resolution of the model output, or comparing changes in vertically resolved ozone with changes in total column ozone. We will investigate how changes in ozone due to ODS and greenhouse gases are geographically distributed and how well this is captured by existing ground-based networks.

Similarly, simulations into the future (until the end of the 21st century) will be used to assess what the expected changes in ozone and related trace gases are under a given climate change / emission scenario and how this depends on geographical coverage and vertical resolution of the simulated observations. This part of the work will thus primarily address gaps in terms of measurement coverage and representativeness, as well as gaps in additional parameters needed to attribute long-term changes of ozone and related trace gases.

4. References

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List of Acronyms

AERONET	Aerosol Robotic Network (aeronet.gsfc.nasa.gov)
AIRS	Atmospheric Infrared Sounder satellite instrument
AOD	Aerosol optical depth
BIRA	Belgian Institute for Space Aeronomy (www.aeronomie.be)
CCM	Chemistry climate model
CCMI	Chemistry Climate Modeling Initiative (www.met.reading.ac.uk/ccmi)
CTM	Chemistry transport model
ECHAM-HAMMOZ	Aerosol climate model based on the climate model ECHAM
ECHAM/MESSy	Chemistry climate model based on the climate model ECHAM and the Modular Earth Submodel System MESSy
ECMWF	Eurpean Centre for Medium Range Weather Forecasts (www.ecmwf.int)
EMAC	ECHAM/MESSy Atmospheric Chemistry model
EO	Earth observation
FMI	Finish Meteorological Institute
FTIR	Fourier Transform Infra-Red (ground-based) observations
GOSAT	Greenhouse gases Observing SATellite
IASI	Infrared Atmospheric Sounding Interferometer
IGAC	International Global Atmospheric Chemistry project (www.igacproject.org)
KIT	Karlsruhe Institute of Technology (www.kit.edu)
KNMI	Royal Netherlands Meteorological Institute
MACC/CAMS	Monitoring Atmospheric Composition & Climate / Coperrnicus Atmospheric Monitoring System
MOPPIT	Measuement of Pollution in the Troposphere satellite instrumen
MPI BGC	Max Planck Institute for Biogeochemistry (www.bgc-jena.mpg.de)
NDACC	Network for the Detection of Atmospheric Composition Change (www.ndacc.org)
ODS	Ozone Depleting Substance

SCIAMACHY	SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY
SPARC	Stratosphere-troposphere Processes And their Role in Climate (www.sparc-climate.org)
TCCON	Total Carbon Column Observing Network (www.tccon.caltech.edu)
TM3	Global Atmospheric Tracer Model
WCRP	World Climate Research Programme (wcrp-climate.org)