



CoCo2

Prototype system for a
Copernicus CO₂ service

2nd Overview of sensitivity studies performed in CoCo2

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Co-ordinated by





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D9.10 2nd Overview of sensitivity studies performed in CoCO2

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CoCO2: Prototype system for a Copernicus CO₂ service

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monitoring support capacity for fossil CO₂ emissions

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1 Executive Summary

Sensitivity studies, including Observing Systems Simulation Experiments, are important tools for a successful design of the prototype CO₂MVS capacity and especially for the foreseen (pre-)operational service in the Copernicus programme. The CoCO₂ project includes many sensitivity studies distributed over most WPs to assess the impact of various choices (observation networks, modelling, data assimilation) on the produced results. To keep a clear focus on the outcome of the various results, this document summarises the performed studies and outcomes. This second version adds the activities for 2022 on top of the activities during 2021.

2 Introduction

2.1 Background

To support EU countries in assessing their progress for reaching their targets agreed in the Paris Agreement, the European Commission has clearly stated that a way to monitor anthropogenic CO₂ emissions is needed. Such a capacity would deliver consistent and reliable information to support policy- and decision-making processes.

To maintain Europe's independence in this domain, it is imperative that the EU establishes an observation-based operational anthropogenic CO₂ emissions Monitoring and Verification Support (CO₂MVS) capacity as part of its Copernicus programme.

The CoCO₂ Coordination and Support Action is intended as a continuation of the CO₂ Human Emissions (CHE) project, led by ECMWF. In the Work Programme, ECMWF is identified as the predefined beneficiary tasked to further develop the prototype system for the foreseen CO₂MVS capacity together with partners principally based on the CHE consortium. In addition, ECMWF will continue some of the work initiated in the EU-funded VERIFY project (<https://verify.lsce.ipsl.fr/>) as well.

The main objective of CoCO₂ is to perform R&D activities identified as a need in the CHE project and strongly recommended by the European Commission's CO₂ monitoring Task Force. The activities shall sustain the development of a European capacity for monitoring anthropogenic CO₂ emissions. The activities will address all components of the system, such as atmospheric transport models, re-analysis, data assimilation techniques, bottom-up estimation, in-situ networks and ancillary measurements needed to address the attribution of CO₂ emissions. The aim is to have prototype systems at the required spatial scales ready by the end of the project as input for the foreseen Copernicus CO₂ service element.

Putting together the building blocks of the CO₂MVS requires extensive testing of all the components as well as the integrated end result. CoCO₂ is therefore using various forms of sensitivity studies to test and illustrate the impact of specific configurations on the estimated emissions. In the Work programme text, specific reference was made to the use of Observation System Simulation Experiments (OSSEs). OSSEs in the context of satellite systems are defined as follows: *An OSSE uses computer models to test different designs of new satellite systems before their instruments are actually built or deployed, and to compare the performance of the new satellites against current observing platforms. The results can help to guide the design of new instruments and to determine if a new satellite platform will be cost-effective.* OSSEs can be computationally expensive and only address part of the overall system. CoCO₂ therefore uses a variety of sensitivity study set-ups that not only address the requirements for the observation component of the CO₂MVS, but also the requirements for

some of the other components. This document provides an overview of the preparation for and results from the various sensitivity studies in CoCO₂.

2.2 Scope of this deliverable

2.2.1 Objectives of this deliverables

During the review of the original CoCO₂ proposal, reviewers commented that the continued prioritisation of the sensitivity studies and the Observing Systems Simulation Experiments will be important to the achievement of the objectives. The proposal includes many sensitivity studies distributed over most WPs to assess the impact of various options (observation networks, modelling, data assimilation) on the produced results. These are indeed very important for a successful design of the prototype and especially the foreseen (pre-)operational service in the Copernicus programme. To keep a clear focus on the outcome of the various results, this document summarises the performed studies and outcomes. It is updated at the end of each year resulting in three Deliverables. The current version, D9.10, is the second version of the document (for the first version, see D9.9).

2.2.2 Work performed in this deliverable

As per the Description of the Action, the work performed included interaction with WP leads to summarise the relevant activities within each Work Package during the first year of the project.

2.2.3 Deviations and counter measures

No deviations were encountered.

3 Related work in 2021

3.1 WP2 - Prior and ancillary information

The work in WP2 does not include specific sensitivity studies but supports studies in other work packages. The global and regional emission data sets are important inputs for the various nature runs, that are setting baselines for the planned sensitivity studies. The Mosaic data set, which is under development, will allow testing the impact of more detailed regional emission data sets compared to the globally consistent but coarser global data set.

3.2 WP3 - Global Modelling and data assimilation

The work in WP3 is primarily focused on further development of the global modelling and data assimilation system with a clear emphasis on ECMWF's IFS system, which is already at the core of the global Copernicus Atmosphere Monitoring Service (CAMS) services. However, various tests and sensitivity studies will be carried out, also including other global systems. Examples are the sensitivity of the length of the data assimilation window on the emission estimates or the sensitivity of the modelling of atmospheric CO₂ to specific choices/assumptions in the land surface modelling. In addition, the work package will provide nature runs based on the improved global system that can be used in sensitivity studies in other work packages. Most of the foreseen work is in progress or planned for the next two years, but an overview of activities so far for the work package in general can be found in D3.1.

3.3 WP4 - Local and regional modelling and data assimilation

The future CO₂M satellites will be able to identify the plumes of strong point sources and clusters of sources (e.g., cities, industrial complexes) with a horizontal resolution of 2 km x 2 km. In order to use this information in atmospheric inversion systems, the underlying atmospheric transport models should be able to resolve the plumes and reproduce their basic properties. Currently, large uncertainties exist regarding the ability of atmospheric transport models to describe individual observed plumes. Moreover, simulation results are sensitive to different model settings such as resolution, boundary layer and advection schemes, and to the representation of the source, such as its temporal variability and injection height in the case of stack emissions. Moreover, models that run on regional scale, are also sensitive to meteorological forcing.

In order to test the current high-resolution transport models, WP4 has defined several test cases that are relevant for emission verification. These cases are meant as benchmark cases that are simulated by an ensemble of high-resolution models including Large Eddy Simulation (LES) and regional non-hydrostatic atmospheric transport models with grid spacings ranging from 50 m to 6 km. The simulations will not only include CO₂, but also co-emitted species like NO₂ and CO, simulated with full or simplified linear chemistry. Cases will be presented for which suitable validation data (satellite, ground-based, (aircraft) campaigns) is available.

Deliverable D4.1 has documented the planned case studies, the participating modelling systems, and available observational datasets to evaluate the simulations. This document will then guide the experimentation with the various modelling systems; first results for the Jämschwalde powerplant have been gathered to test and refine the simulation setups.

3.4 WP5 - Connecting scales and uncertainties

A cornerstone of the multi-scale CO₂MVS prototype is the use of ensembles for the exchange of statistical information between global and local inversion systems. WP5 has focused on two main activities, both of which rely on posterior ensembles generated by the global Integrated Forecasting System (IFS) at ECMWF as well as the regional systems:

1. Use of the global IFS posterior ensemble as set of boundary conditions for the regional inverse models, in order to quantify the impact of uncertainties in those boundary conditions on the regional top-down estimates.
2. Combination of the global IFS posterior ensemble with posterior ensembles from regional emission products to assimilate the latter as observations in the global inversion prototype.

During 2021, work has focused on extending the existing Ensemble of Data Assimilation (EDA) framework of the IFS to integrate perturbations of both the 3-dimensional atmospheric composition state and the emissions in the posterior ensemble. The extended EDA framework can be used to create flow-dependent errors for use in the global inversion system as well as in the regional and local systems. It also allows to perform Observation System Simulation Experiments later in the project. A description of the work carried out so far is presented in D5.7.

Another activity in WP5, also documented in D5.7, is the extension of the VERIFY Community Inversion Framework (CIF) to the models used in CoCO₂. Accurately assessing uncertainties originating from the use of different transport models and configurations needs to be carried out using a common system with all inversion steps identical, with the exception of the transport. At the time of writing of the present report, the following models are fully integrated in the CIF and are usable for later assessment of transport uncertainties: CHIMERE, LMDZ, FLEXPART, TM5, and WRF-Chem. Discussions with partners to establish a clear inversion protocol, to use the CIF with different models and later deduce a quantification of transport uncertainties have started in autumn 2021. The purpose is to coordinate with other WPs and

decide of a relevant inversion window consistent with other inversions carried out in other tasks.

WP5 also contains a specific task to assess the impact of various design options for the CO₂MVS and has built in some flexibility to respond to questions from the CO₂ Task Force (T5.5). The global CCFFDAS provided a contribution to the CO₂ Task Force report entitled “Recommendation on Constellation Size of the CO₂M Mission”. The contribution quantified the effect of adding satellites to the CO₂M constellation for an exemplary week in June on sectoral fossil fuel emissions from five countries (Australia, Brazil, China, Germany, and Poland). It detailed that “each additional satellite in the constellation achieves a further reduction in posterior uncertainty of country-scale sectoral fossil fuel emissions. As the electricity generation sector is relatively well-constrained by prior information, at country scale the main impact of atmospheric XCO₂ and in situ CO₂ observations was on the posterior uncertainties of the fossil fuel emissions from other sectors. A local CCFFDAS system was employed to assess the constraint of simulated CO₂M images of XCO₂ and of the NO₂ column for an overpass on February 3, 2008, on fossil fuel emissions from power plants and all other sectors (called “the other sector”) at varying degrees of spatial aggregation over the 24 hours preceding the emission. It explored the sensitivity to the random uncertainty in NO₂ observations by analysing five cases. More details can be found in section 3.5 of D5.7. In addition, a series of experiments using TROPOMI CH₄ observations was performed with the CarbonTracker Europe-CH₄ inversion system. The experiments differ in the retrieval product assimilated. One was based on the operational algorithm and one on the Weighting Function Modified Differential Optical Absorption Spectroscopy (WFM-DOAS or simply WFMD). An inversion based on the in-situ network was used as a benchmark. Results show that significant differences still exist when using different (satellite) observation products. More details in D5.7.

Finally, the impact of transport model uncertainties on atmospheric CO₂ inversions was tested through a set of inversions that differ only by their atmospheric transport models. Findings are described in Section 3.6.1 of D5.7.

3.5 WP7 - Observations

One specific task in this work package, Task 7.3 Identification of gaps in the currently available in-situ observations and ancillary data, will address in-situ observational needs with a design study for a future comprehensive in-situ network. This will link directly with Task 5.5, which aims to perform quantitative network design studies addressing the in-situ network (i.e., type and coverage of observations) and the inclusion of radiocarbon observations. The task has not been active yet, because it needs the results from Task 7.1 (Definition of requirements for in situ observations) and Task 7.2 (Identification of data providers) to confront the data needs documented in Task 7.1 with the currently available data streams documented in Task 7.2. It is expected that a mismatch will be apparent, which may take the form of insufficient measurement coverage, or limited timeliness and/or quality control of the required measurements for use in an operational context. Entirely missing data streams, representing scales and variables that are currently not observed, may also be identified. Thus, the outcome of this task will not only be the documentation of the gaps themselves but will also lead to recommendations for how to cost-effectively close these gaps for the in-situ network and radiocarbon measurements.

4 Related work in 2022

4.1 WP2 - Prior and ancillary information

As stated above, the work in WP2 does not include specific sensitivity studies but supports studies in other work packages. The global and regional emission data sets are important inputs for the various nature runs, that are setting baselines for the planned sensitivity studies. The Mosaic data set, which was finalised in 2022, will allow testing the impact of more detailed

regional emission data sets compared to the globally consistent but coarser global data set. In addition, the prior uncertainty dataset related to the European and global prior emission datasets (PED) for the year 2018 was delivered as D2.6. This provides an overview of the developed methodology to estimate prior uncertainties in the aggregated PED starting from a detailed set of uncertainties. This also includes the estimation of gridded uncertainties and spatial error correlation lengths. These uncertainties are important inputs to all inverse modelling and data assimilation studies in the project.

4.2 WP3 - Global Modelling and data assimilation

The work in WP3 is primarily focused on further development of the global modelling and data assimilation system with a clear emphasis on ECMWF's IFS system, which is already at the core of the global CAMS services. However, various tests and sensitivity studies will be carried out, also including other global systems. Examples are the sensitivity of the length of the data assimilation window on the emission estimates or the sensitivity of the modelling of atmospheric CO₂ to specific choices/assumptions in the land surface modelling. In addition, the work package will provide nature runs based on the improved global system that can be used in sensitivity studies in other work packages. Most of the foreseen work is in progress or planned for the final year.

4.3 WP4 - Local and regional modelling and data assimilation

In order to test the current high-resolution transport models, WP4 defined several test cases that are relevant for emission verification in the first year of the project (D4.1). These cases are meant as benchmark cases that are simulated by an ensemble of high-resolution models (50 m – 6 km). During 2022, an assessment of five high-resolution transport models (COSMO-GHG, ICON-ART, LOTOS-EUROS, MicroHH, WRF-CHEM) to simulate the plume from three large coal-fired power stations, a steel plant, and three (conglomerate) city plumes has been carried out. The simulated results have been compared against observations (in-situ airplane observations for two power plant cases and one city case; in-situ ICOS and other high-precision CO₂ measurements for two city cases; 43 NO₂ measuring stations for a city case; TROPOMI images for all cases), as well as amongst each other. A comprehensive deliverable report has been produced and is available as D4.2. Furthermore, a library of total column CO₂ plumes has been generated by mapping the output of all model simulations to a common 2 km x 2 km grid consistent with the resolution of the future CO2M satellites. This data set has been published on zenodo (doi:10.5281/zenodo.7448144) and may serve as a basis for future OSSE simulations.

Another activity has been the benchmarking of six different light plume detection and quantification methods using synthetic SMARTCARB CO₂ and NO₂ observations from the future CO2M satellites produced in the ESA project SMARTCARB. The methods were tested in a number of different configurations to evaluate their sensitivity to the effects of clouds, wind uncertainty, and the advantage of using NO₂ observations from CO2M in addition to CO₂. Benchmarking consists of analysing individual CO2M overpass estimates as time series over one year as well as annual and seasonal emission estimates. Specific attention has been given to analysing the trade-off between the quality and quantity of the flux estimates by filtering the data with more or less stringent quality thresholds. At the time of writing of this document, the work was still being finalised with the aim to produce a full deliverable report (D4.4) by the end of February 2023.

4.4 WP5 - Connecting scales and uncertainties

During 2022, work has continued on extending the existing Ensemble of Data Assimilation (EDA) framework of the IFS to include perturbations of both the atmospheric composition observations and the prior emissions, on top of the existing perturbations of the meteorological

observations and the model physics. This extended EDA configuration is now technically working and is being used for longer experimentation. The extended EDA framework can be used to create flow-dependent errors for use in the global inversion system as well as in the regional and local systems. It also allows to perform Observation System Simulation Experiments in the final year of the project.

In Task 5.3, activities rely on the continued developments of the Community Inversion Framework (CIF). In 2022, these developments included dedicated efforts on integrating satellite observations in inversions, with regards to the processing of huge datasets and accelerating computations, as well as the integration of inversion methods beyond the variational approach (CIF now includes ensemble filter methods). Progress was stalled on two main axes due to technical issues. The first one concerned the migration of the ECMWF archive to new data servers in Bologna; the migration delayed work in T5.1 which will be used for sensitivity analysis of regional inversions with regards to meteorological forcing and boundary conditions. The second bottleneck came from the upgrade of TM5 to TM5-MP. Due to library issues, TM5-MP is still not coupled to CIF, which limits the options in terms of inter-comparisons. The integration of ensemble of perturbed meteorology and boundary conditions resumed in December 2022 and will be used in connection to T5.1 to systematically assess the impact of uncertain meteorology and boundary conditions on regional CO₂ inversions.

In Task 5.4, the progress proceeded slower than planned because of a change in personnel at WP leader VUA, which took from the beginning of March to mid-October 2022 to repair. Since then, the work concentrated on the construction of a simulated CO₂M dataset for use within and outside of this WP. Orbits with the coordinates of a year of global CO₂M data were made available by EUMETSAT. This dataset is being extended with information on total column CO₂, clouds, and estimated random and systematic errors of XCO₂ retrievals from CO₂M. To compute errors, we make use of the error parameterization of Buchwitz et al. (2013) updated with results from the CO₂M end-to-end simulator developed at SRON. Currently, all inputs have been collected (AOD and CO₂ from CHE Lotos-Euros simulations; surface reflectance and AOD from MODIS; climatological COD and cirrus height from the CarbonSat L2e database). The processing of the CO₂M datasets has started but needs further optimization to improve the processing efficiency of the large datasets involved.

In Task 5.5, the series of experiments using TROPOMI CH₄ observations with the CarbonTracker Europe-CH₄ inversion system that had already been performed during the first year of the project have been extended to also investigate the impact of assimilating a new Lower Troposphere CH₄ product derived from GOSAT as compared to the standard GOSAT product. More details on this will be provided in D5.5.

In Task 5.6, submissions to the European methane inversion intercomparison were collected from groups within and outside of the CoCO₂ consortium (currently 8 submissions in total). Participants made use of an experimental protocol that we updated from an existing VERIFY protocol and input database. Software was developed for reading, visualizing, and analyzing the output that we received, with help of the participants in case the processing of output raised questions about units, coordinates, etc. The results have been presented at the Transcom workshop in Wageningen (16-17 Sept 2022). The results show a sizeable inter-model spread in the adjustments to the common set of a priori fluxes needed to bring the models in agreement with the measurements. These adjustments in European emission patterns are very similar in the beginning and end of the multi-year time window of the experiment, pointing to the importance of systematic differences between models and/or inversion methods that were used. Some adjustments are robust across models, such as increased emissions in the Benelux region and reductions in Italy. The latter may have to do with the choice of geological emission dataset that was used as a priori. Consistency checks are being carried out to identify possible remaining issues in the submissions, such as comparisons against independent data and a comparison of domain integrated fluxes. The status of the experiment will be presented at the WMO IG3IS stake holder meeting (Geneva, 2 – 3 February 2023).

For CO₂, the study on the impact of the transport model uncertainties on regional atmospheric CO₂ inversions has been extended to also cover aspects of background information (lateral boundary conditions) as well as the inversion system used, here in particular the form of the prescribed prior error covariance for the terrestrial fluxes. For this an ensemble of in total eight inversions were conducted using combinations of a) inversion system (LUMIA vs CSR), b) background information (provided by applying the global transport models TM3 and TM5) and c) mesoscale transport model (FLEXPART vs STILT).

5 Conclusion

This deliverable provides an overview of the sensitivity studies, and their preparation, carried out across the various work packages in CoCO₂. It emphasizes the importance of these sensitivity studies for the design of the CO₂MVS and makes it easier to find the relevant Deliverables that describe the various studies in more detail. In this second version, activities performed during 2022 have been added to those already described for 2021. A final version will add the activities that will take place during 2023.

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