CoCO2

Prototype system for a Copernicus CO_2 service

Fitness for Purpose Document

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CoCO2: Prototype system for a Copernicus CO_2 service

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1. Introduction

The European Commission is establishing an operational observation-based anthropogenic CO_2 emissions monitoring and verification support capacity (CO2MVS) as part of its Copernicus Earth Observation programme. Demonstrator systems for this CO2MVS are being developed in the Prototype System for a Copernicus CO_2 service (CoCO2) project.

In its information to the 1st Global Stocktake entitled *Data contribution of the European CoCO2 project to the first Global StockTake* (deliverable D6.5), CoCO2 introduced data from five demonstrator systems, each exploring and prefiguring different aspects of the future CO2MVS. The first three are specifically about fossil fuel emissions:

- **local** large fossil fuel CO_2 emissions estimated from observed CO_2 plume cross-sections (section 2);
- **regional** fossil fuel CO_2 emissions estimated by an atmospheric inversion assimilating satellite retrievals of co-emitted species (section 3);
- **global** fossil fuel CO_2 emissions estimated by a Carbon Cycle Fossil Fuel Data Assimilation System (section 4);

The fourth demonstrator data concerns the Agriculture, Forestry, and Other Land Use sector (AFOLU):

- **global** AFOLU emissions estimated by CO_2 atmospheric inversions (section 5);

The fifth demonstrator addresses all global emissions and absorptions synergistically:

- **global** data from an extension of the European Centre for Medium-range Weather Forecasts (ECMWF) Numerical Weather Prediction system (section 6);

The *Functional Requirements Specification Document* (D6.4) describes the codes that have been used to generate Figures 2-7 of D6.5 and explains how the user requirements identified by CoCO2[1] have been addressed from a technical point of view by each demonstrator. The present *Fitness for Purpose Document* explains how these user requirements have been addressed from a scientific point of view. The references for each demonstrator are given directly at the end of the section where it is described.

2. Estimates of large point source fossil fuel CO_2 emissions based on satellite observations

2.1. Introduction

This demonstrator automatically and systematically analyses the data from NASA's second and third Orbiting Carbon Observatories (OCO-2 and -3) scientific missions. It identifies the isolated CO_2 enhancements along the satellite orbits that could correspond to transects of plumes from nearby upwind sources. It then estimates the corresponding emission with a simple plume cross-sectional inversion approach and performs quality control. More specifically, it uses the operational quality-controlled bias-corrected retrievals of the column-average CO_2 dry air-mole fraction (XCO_2) made by NASA’s Atmospheric CO_2 Observations from Space (ACOS) algorithm.

[1] https://www.coco2-project.eu/sites/default/files/2022-03/CoCO2-D6-3-V1-0.pdf

2.2. Quality-control of the production chain

The method was developed by Zheng et al (2020) and Chevallier et al (2020, 2022), who were able to demonstrate its skill. In particular, the authors compared their results with a global gridded and hourly inventory. They found that the corresponding OCO emission retrievals explain more than one third of the inventory variance at the corresponding cells and hours. Furthermore, the data was binned at diverse time scales from the year (with OCO-2) to the average morning and afternoon (with OCO-3), resulting in consistent variations of the median emissions, indicating that the retrieval-inventory differences (with standard deviations of a few tens of percent) are mostly random and that trends can be calculated robustly in areas of favourable observing conditions, when there is enough data.

Since the implementation of the algorithm is very similar to the one of Chevallier et al (2022), the analysis of temporal variability has not been repeated. The main change consisted in replacing the Emissions Database for Global Atmospheric Research (EDGAR), v6.0, used for the enhancement selection, by the coal-fired power plant and steel plant data from the Global Energy Monitor (https://globalenergymonitor.org/). The advantage of this database is the monitoring of the plants being much closer to real time than EDGAR, i.e., months behind real time rather than years. The new database is restricted to coal-fired power plants and steel plants, however Chevallier et al. (2022) noticed that the isolated enhancements selected in the OCO data are originated mostly from large emitters in the power-industry sector and, to a smaller extent, in the combustion-for-manufacturing sector; the other sectors, like road transport, had a smaller share. By using the Global Energy Monitor data rather than EDGAR, we also lose the sub-annual temporal variability of this dataset, in particular for emissions from the power sector, but we assume that when an OCO sees a coal-fired power plant plume, this plant operates at the maximum of its capacity.

The evolution of the production chain and the data that it generated for D6.5 have been quality-controlled by a comparison between the retrieved emissions and those of the Global Energy Monitor accumulated in the footprint of each emission retrieval, assuming a capacity factor of 100 % at observation time. This comparison is shown in **Figure 1** in the case of the OCO-2 data, v11. 278 enhancements have been selected by the automated algorithm. The cloud of points shows an overall distribution along the bisector, with a slope of 1.1 and an r^2 of 0.47. The figure actually displays the cloud of points with both axes on logarithmic scales because the retrieval values are distributed heterogeneously over three orders of magnitude. If we take the logarithm of the emissions, as is done in practice in the figure, r^2 increases up to 0.54; the slope is then 0.8. There is usually more than one large emitter in the plume footprint and the agreement is for the total, not for one specifically. For OCO-2 v10 data, 304 enhancements have been selected by the automated algorithm, over a longer period of time than that allowed by v11. The r^2 is of 0.44 and 0.42, without and with logarithm scale, respectively. For OCO-3 data, 65 enhancements have been selected by the automated algorithm, in which the resulting r^2 is of 0.42, either with or without logarithm scale.

These r^2 values are larger than those reported in Chevallier et al. (2022) when comparing the emission retrievals to EDGAR, despite the lack of temporal variability in the plant emissions and the lack of neighbouring emissions from other sectors, when using the Global Energy Monitor.

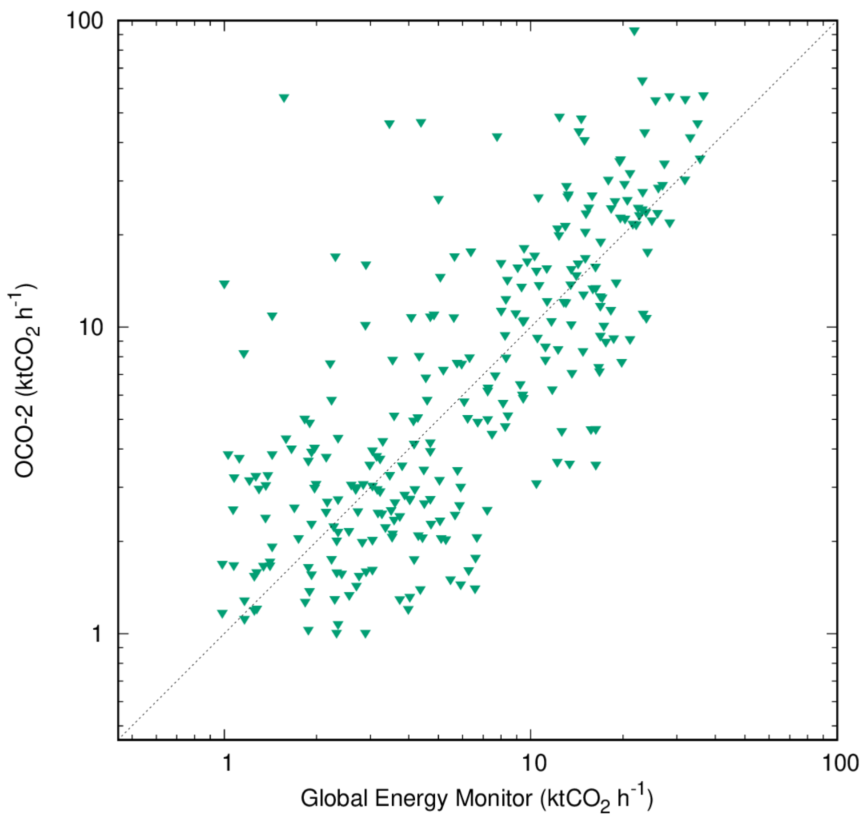

Figure 1 – Retrieved emission values for OCO-2 v11 data versus the values inferred from https://globalenergymonitor.org/. The black dots form the bisector. Units in $ktCO_2h^{-1}$, and both axes on logarithmic scales

2.3. Link with the user requirements

This demonstrator addresses the first Guiding question by the Subsidiary Body Chairs for the Technical Assessment component of the first Global Stocktake[2]: *What is the collective progress in terms of the current implementation of, and ambition in, mitigation actions towards achieving the goals defined in Articles 2.1(a)1 and 4.12 of the Paris Agreement?*

Indeed, its data track high-emission hot-spots over the globe with low latency over time. The small swath of the OCO instruments together with frequent unfavourable observation conditions (e.g., restrictions on insolation, on cloud and aerosol loading) hamper systematic monitoring. Our emission retrievals also correspond to values aggregated in space, in time and along sectors, with a composition that varies with the wind. Their uncertainty is large, with standard deviations of a few tens of percent, but spatial and temporal patterns are found to be realistic when enough data can be aggregated together to damp the random noise. With current instruments, it mostly serves to monitor the trend of the high-emission hot-spots in regions that are wellobserved by the two OCOs.

2.4. References

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[2] https://unfccc.int/sites/default/files/resource/Draft%20GST1_TA%20Guiding%20Questions.pdf

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3. Estimates of fossil fuel emissions from regional inversions using co-emitted species

3.1. Introduction

The sequence of computations implemented by Fortems-Cheiney and Broquet (2022) that is used for the estimate of the national-scale fossil fuel CO_2 ($FFCO_2$) emissions in Europe and for the generation of Figures 3 and 4 of the CoCO2 submission to the GST consists in:

1) the atmospheric inversions of maps of the NO_x or CO emissions over Europe during 2005-2021 at 1-day and 0.5° resolution. These inversions are based on the coupling between the variational mode of the Community Inversion Framework (CIF, Berchet et al., 2021), a configuration for Europe of the CHIMERE regional atmospheric chemistry transport model (Menut et al., 2013) and the adjoint code of this model (Fortems-Cheiney et al., 2021). The NO_x and CO inversions assimilate respectively atmospheric NO_2 and CO products from spaceborne instruments: the OMI-QA4ECV-v1.1 (Boersma et al., 2017) or TROPOMI-PAL (Eskes et al., 2021) NO_2 Tropospheric Vertical Column Density (TVCD) and the MOPITT-v8J (NIR-TIR) CO surface product (Deeter et al., 2019). The inversions apply corrections to a "prior" information on the emissions: maps of anthropogenic emissions from an inventory of the European NO_x, CO, and CO_2 emissions by the TNO organisation (the TNO-GHGco-v3 inventory, Super et al., 2020) and maps of biogenic emissions of NO_x from the MEGAN model (Guenther et al., 2006).

2) the conversion of the daily maps of NO_x or CO anthropogenic emissions from these inversions into estimates of the fossil fuel CO_2 ($FFCO_2$) emissions at the national and monthly scale for five large groups of sectors of emitting activities. This conversion relies on the sectoral maps of emissions from the three species and, implicitly, on the emission ratios between the species for each sector, country, and month from the inventory by TNO.

3.2. Quality-control of the production chain

Traditional internal diagnostics of the variational inversions are used to evaluate the atmospheric inversions of maps of the NO_x or CO emissions. In particular, the norm of the gradient of the cost function *J*, whose minimum is searched for with the iterative limited-memory quasi-Newton minimization algorithm M1QN3 (Gilbert and Lemaréchal, 1989) used by the inversions to find the optimal emission maps is reduced by more than 90 % in all cases.

The level of reduction of the misfits to the assimilated data by the inversion (compared to the misfits obtained when using the prior estimate of the emissions) is also analysed, even though it cannot be taken as a direct index of the quality of the inversions. In general, this reduction is much larger over polluted areas (with a reduction of the biases of a tens of % for a given month over such areas).

However, there is currently no estimate of the uncertainties in the NO_x and CO emission maps from these inversions. Such uncertainties emerge from the combination of the uncertainties in the atmospheric chemistry-transport modelling, in the satellite NO_2 and CO products, and in the prior estimate of the emissions. While different techniques (e.g., Monte Carlo ensemble techniques) allow, in theory, to derive estimates of these uncertainties for variational inversions, the corresponding computational cost is large and raises challenges.

Finally, there is no real quality-control regarding the conversion of the daily maps of NO_x or CO anthropogenic emissions from these inversions into estimates of fossil fuel CO_2 emissions at the national, monthly, and sectoral scale. In practice, the relatively small differences between the maps and budgets of NO_x and CO emissions from the inversions and from the TNO-GHGco-v3 inventory make the $FFCO_2$ estimates from the sequence of inversions and conversion quite consistent with the inventory. The NOx-to-$FFCO_2$ and CO-to-$FFCO_2$ emission ratios from the TNO-GHGco-v3 inventory that are used for the conversion bear uncertainties, but there is a lack of precise characterization for these uncertainties.

3.3. Link with the user requirements

This demonstrator addresses the first Guiding question by the Subsidiary Body Chairs for the Technical Assessment component of the first Global Stocktake[3]: *What is the collective progress in terms of the current implementation of, and ambition in, mitigation actions towards achieving the goals defined in Articles 2.1(a)1 and 4.12 of the Paris Agreement?*

It provides national budgets of $FFCO_2$ emissions in Europe aggregated over 5 large groups of sectors of activity, at annual to 1-month scale and over more than 15 years. The current product bears large uncertainties, however, the analysis of the results from this demonstrator highlight the capability to assimilate satellite data on co-emitted species for the estimation of fossil fuel CO_2 emissions and the overall consistency between these datasets and current inventories. The relevance of this assimilation will grow with the availability and co-assimilation of data at high spatial resolution from satellite missions dedicated to fossil fuel CO_2 (such as CO2M) with the regular improvement of satellite products and spatial resolution for all species. Furthermore, this demonstrator will also benefit from the precise characterization of the uncertainties in the spatial distribution and emission ratios in pollutant and spatialized and temporalized inventories of greenhouse gases.

[3] https://unfccc.int/sites/default/files/resource/Draft%20GST1_TA%20Guiding%20Questions.pdf

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4. Estimates from a Carbon Cycle Fossil Fuel Data Assimilation System

4.1. Introduction

The Carbon Cycle Fossil Fuel Data Assimilation System (CCFFDAS, Kaminski et al., 2022) pursues an innovative approach to the estimation of fossil fuel emissions in that it combines top-down (inverse modelling) and bottom-up (forward modelling) of sectoral fossil fuel emissions and of the terrestrial biosphere. The inclusion of such process-based forward models ensures consistency of the posterior flux estimates with process understanding as incorporated in the underlying models. It also enables the CCFFDAS to complement atmospheric concentration measurements with additional data streams, e.g., from emission statistics, from satellite-observed night-light intensity, on vegetation activity, or climate data in the estimation procedure. This feature extends the capabilities of traditional atmospheric inverse modelling and data assimilation systems.

4.2. Quality control of the production chain

The system relies on well-tested component models. Preliminary tests on the production chain include the inspection of residuals, in particular of simulated country-scale emissions against reported national totals, and of the deviation from prior information, particularly of emissions from power plants. Further standard diagnostics, such as the norm of the cost function gradient, are also inspected.

4.3. Link with the user requirements

This demonstrator addresses the first Guiding question by the Subsidiary Body Chairs for the Technical Assessment component of the first Global Stocktake[4]: *What is the collective progress in terms of the current implementation of, and ambition in, mitigation actions towards achieving the goals defined in Articles 2.1(a)1 and 4.12 of the Paris Agreement?*

and the fourth one: *How adequate and effective are the current mitigation efforts and support provided for mitigation action towards achieving Articles 2.1(a) and 4.1 of the Paris Agreement?*

With respect to the user requirements, identified by CoCO2[5], the CCFFDAS addresses by construction the user requirement of disentangling fossil fuel CO_2 emissions and natural land-atmosphere CO_2 exchange fluxes. Likewise, it differentiates the fossil fuel CO_2 emissions into sectoral emissions (in the setup currently used two: electricity generation and the rest. The posterior fossil fuel emission estimates are provided on a global 0.1 º grid (this is, however, dependent on the input data used and can therefore also be higher), and thus provide relevant information for supporting mitigation efforts from local to national to global scale. Furthermore, it is worth noting that the CCFFDAS system can be operated in two modes: the synergistic mode, which includes (IEA or other) sectoral national emission totals as an observation used in the model parameter calibration; and alternatively, in verification mode, i.e., without using the IEA sectoral national emission totals. This latter mode provides emission estimates that are largely independent of data used for the bottom-up estimation of emissions, thus allowing to address another user requirement.

4.4. References

[4] Asefi-Najafabadi et al. (2003, https://doi.org/10.1002/2013JD021296)
[5] https://www.coco2-project.eu/sites/default/files/2022-03/CoCO2-D6-3-V1-0.pdf

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5. Estimates of AFOLU emissions from CO_2 atmospheric inversions

5.1. Introduction

This demonstrator relies on the time series of the sum of emissions and removals estimated by the already operational atmospheric inversions of the Copernicus Atmosphere Monitoring Service (CAMS)[6].

5.2. Quality control of the production chain

Compared to the initial study of Chevallier (2021), the CAMS products and the UNFCCC Common Reporting Format tables (CRF) have been updated, with each data source having its own quality-control procedure. Correction terms have been added to tentatively account for the lateral transport of carbon from crop trade and river flow using data from the literature and living databases (Ciais et al. 2022, Deng et al. 2022), however these terms are difficult to validate.

The only specific evaluation that has been performed in this report concerns the statistical consistency between the two CAMS products used. When assuming that the two inversions are independent (given the very different nature of their assimilated data, and the large volume of the satellite data assimilated by one of them), the reduced chi-squared statistics of the series of 70 differences between the two inversions (10 Parties times 7 years) is 0.88. This value was obtained without any new tuning, being slightly larger than that reported by Chevallier (2021) on a shorter time series and with previous CAMS products. The difference between the two inversions seems to be fairly explained by their error bars, which strengthens our confidence in the realism of the CAMS statistical models.

5.3. Link with the user requirements

This demonstrator too addresses the first Guiding question by the Subsidiary Body Chairs for the Technical Assessment component of the first Global Stocktake[7]: *What is the collective progress in terms of the current implementation of, and ambition in, mitigation actions towards achieving the goals defined in Articles 2.1(a)1 and 4.12 of the Paris Agreement?*

It provides numbers that are directly comparable to aggregated numbers from the National Inventory Reports (NIRs) for the AFOLU sector, despite remaining conceptual differences or ambiguities (e.g., temporal support, spatial perimeter, scope of the processes) between the NIRs and what the atmosphere sees. It also provides robust associated uncertainty statistics.

[6] https://ads.atmosphere.copernicus.eu/cdsapp#!/dataset/cams-global-greenhouse-gas-inversion
[7] https://unfccc.int/sites/default/files/resource/Draft%20GST1_TA%20Guiding%20Questions.pdf

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6. Estimates of CH_4 emissions from the extended Copernicus Atmosphere Monitoring Service global monitoring system

6.1. Introduction

This demonstrator is based on an extension of the Integrated Forecasting System (IFS) 4D-variational data assimilation system used operationally at ECMWF. It consists of including the optimisation of surface CH_4 fluxes jointly with the atmospheric CH_4 concentrations and meteorological variables.

6.2. Quality control of the production chain

The prescribed prior errors in CH_4 emissions have a significant impact on the quality of the posterior emission product. In our inversion, prior errors are selected based on sensitivity experiments, where the performance of the emission optimisation, in terms of forecasted 3D CH_4 concentrations, using different prior error assumptions, is evaluated against satellite observations (McNorton et al., 2022). Additionally, after selecting optimal prior errors, the quality of the 4D-Var joint state/emission inversion is evaluated by running the IFS model starting from the optimal state and comparing the simulated XCH4 columns with measurements from 16 Total Column Carbon Observing Network (TCCON) sites (Wunch et al., 2011). TCCON averaging kernels were applied to model profiles, as described in Massart et al. (2016). Results show improved performance when including flux scaling factors in the control vector compared with only optimising the initial 3D-state (McNorton et al., 2022) (see **Figure 2**). When evaluating XCH4 concentrations simulated with optimised emissions using the optimal prior errors, the lowest all-site average standard error (6.8 ppb) and absolute mean bias (7.52 ppb) were found.

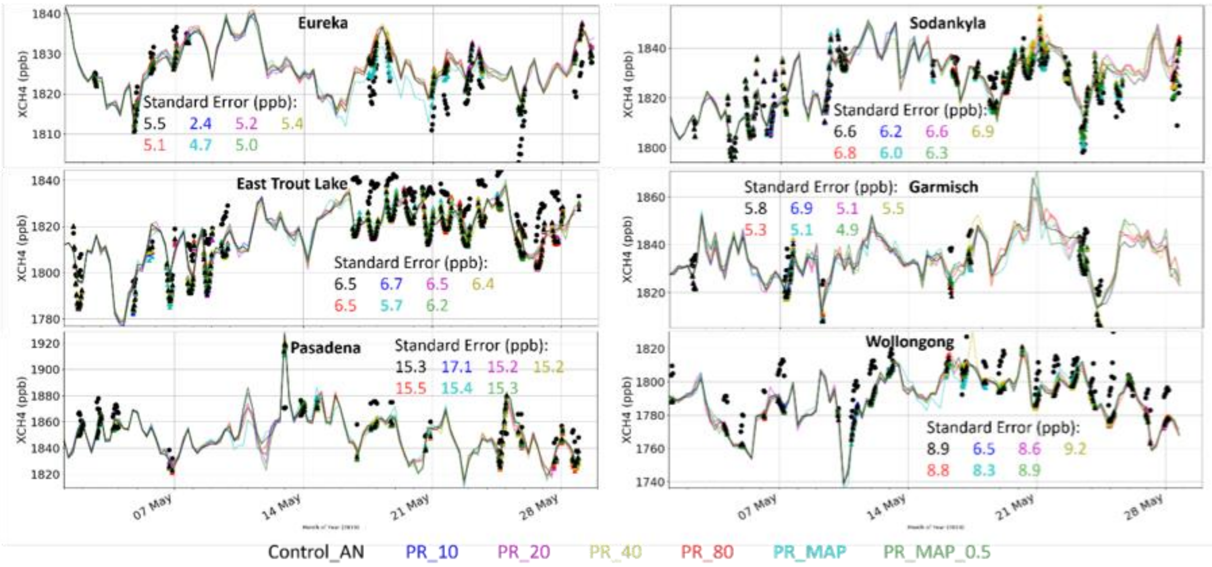

Figure 2 – Comparisons of XCH4 from inversions using 6 different prior uncertainties and 1 where only the initial 3D-state is optimised (Control_AN) with a subset of 6/16 TCCON sites for May 2019 with standard error values given.

6.3. Link with the user requirements

This demonstrator addresses the first Guiding question by the Subsidiary Body Chairs for the Technical Assessment component of the first Global Stocktake[8]: *What is the collective progress in terms of the current implementation of, and ambition in, mitigation actions towards achieving the goals defined in Articles 2.1(a)1 and 4.12 of the Paris Agreement?*

It provides national budgets of CH_4 emissions from monthly to yearly time scales, being directly comparable to aggregated numbers from the National Inventory Reports (NIRs).

6.4. References

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Document History

Version	Author(s)	Date	Changes
1.0	All authors	25/01/2023	Initial version
1.1	F Chevallier	07/02/2023	Inclusion of the reviewers' suggestions

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