D7.2:

Book of *in situ* data requirements V2

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Co-ordinated by ECMWF

CoCO2

Prototype system for a
Copernicus CO_2 service

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Dissemination Level:	Public
Author(s):	Julia Marshall (DLR)
Date:	27/01/2023
Version:	1.0
Contractual Delivery Date:	31/12/2022
Work Package/ Task:	WP7/ T7.1
Document Owner:	DLR
Contributors:	ICOS-ERIC for carrying out the surveys, with responses from ECMWF, EMPA, CEA, MPI-BGC, TNO, LUND, VUA, AGH, BSC, CNRS, DWD, FMI, iLab, and UEDIN
Status:	Final/Public

CoCO2: Prototype system for a Copernicus CO$_2$ service

Coordination and Support Action (CSA)
H2020-IBA-SPACE-CHE2-2019 Copernicus evolution – Research activities in support of a European operational monitoring support capacity for fossil CO2 emissions

Project Coordinator: Dr Richard Engelen (ECMWF)
Project Start Date: 01/01/2021
Project Duration: 36 months

Published by the CoCO2 Consortium

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The CoCO2 project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 958927.

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1 Executive Summary

This deliverable is the second iteration of the report on the *in situ* and ancillary data requirements of the prototype of a Copernicus CO_2 service being developed within the CoCO2 project. The goal of such a service is to provide timely estimates of carbon dioxide fluxes informed by atmospheric measurements, modelling, and additional measurements. This report aims to document the data needs of this system. The documentation of these requirements is a critical step in transitioning the project from a scientific exercise to an operational capacity, enabling the identification of data dependencies and potential weak links in the future provision of timely flux estimates. The data needs across 13 types of *in situ* measurements and 8 types of ancillary data products have been documented. Particular attention was paid to the timeliness requirements of the data, in addition to other specifications such as spatial coverage, temporal resolution, and where the project participants are currently accessing the various data streams.

This report builds upon the previous deliverable D7.1, but was further informed by group interviews with participants of the relevant work packages, which were conducted online.

An analysis of the responses finds that the global integration and attribution work within Work Package 3 has the strictest timeliness requirements, which are currently only clearly met by satellite measurements and the *in situ* measurements of the ICOS network. This may result in the operational assimilation relying predominantly on satellite products as input, with *in situ* data being used primarily for (re-)analyses and regional applications. Additionally, the lack of near-real-time data results in temporal delays in the production of anthropogenic emission inventories in Work Package 2, resulting in the use of temporally extrapolated prior emissions by modelling groups.

This report is the second edition of this document, which is evolving as the project matures. The third and final edition will be produced during the final year of the project.

2 Introduction

2.1 Background

The prototype CO_2 Monitoring & Verification Support (MVS) capacity being developed within the CoCO2 project aims to extract information about anthropogenic greenhouse gas emissions from satellite measurements provided by the constellation of CO_2 sensors that will make up the planned CO2M mission. These satellites will provide imager-type column-integrated measurements of atmospheric CO_2, CH_4, and NO_2 at ~2 km x 2 km resolution with a swath ~250 km wide, enabling the imaging of emission plumes from point sources and hot spots associated with anthropogenic activities, and global coverage to constrain emissions on national scales.

While these satellites are being developed with this application in mind, an integrated system will also require extensive *in situ* and ancillary observations to achieve its proposed objectives. Multiple data streams of *in situ* measurements will play a role here, including, but not limited to, measurements of greenhouse gas fluxes and atmospheric mixing ratios of greenhouse gases. Note that in the context of the Copernicus Programme, *in situ* data refers to measurements made by ground-based, seaborne or airborne sensors, including remote sensing sensors, as well as reference and ancillary data.

These data can be used for a variety of applications within the MVS prototype, each of which comes with a different set of requirements in terms of timeliness, coverage, and precision. In

Pinty et al. (2019), the CO_2 Monitoring Task Force convened by the European Commission documented the needs and high-level requirements for *in situ* measurements that are foreseen in the MVS capacity, and their report (informally referred to as “the Green Report”) has guided the work reported here. Their report identified the following general areas in *which in situ* measurements will be required:

- Calibrating and validating the space component of the MVS capacity,
- Assimilating the data into models and integrating information in the core MVS capacity,
- Validating and further improving physical models that govern the evolution of CO_2 in computer simulations, and
- Evaluating the output generated by the MVS capacity for its end users.

The importance of these data streams is illustrated in the overview diagram of the CoCO2 project, which outlines the structure of the MVS capacity, found in Figure 1. The left pillar of the diagram contains all the observational requirements of the system. The spaceborne measurements are the purview of the space agencies, while the meteorological observations and the assimilation thereof are taken care of by ECMWF. The observational needs that are being documented in this report belong to the other two categories, namely “surface and airborne observations” and “auxiliary observations”.

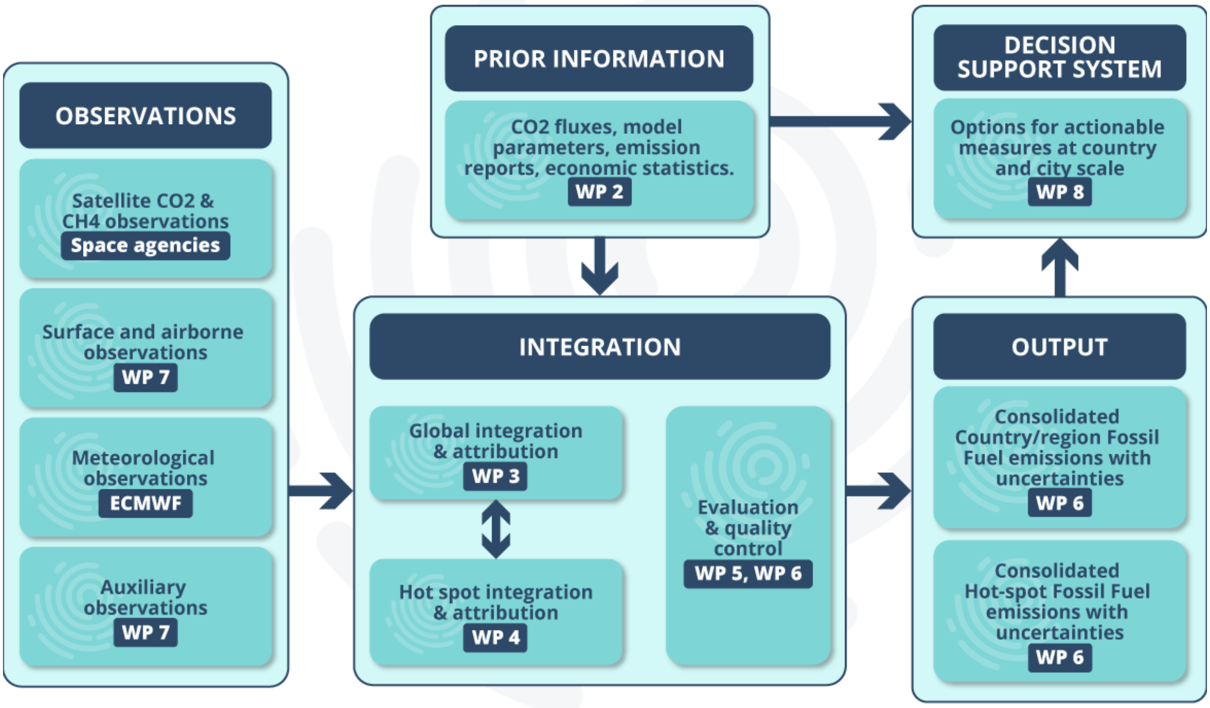


Figure 1: Schematic overview of the CoCO2 project structure, reflecting the structure of the MVS capacity itself. (Source: https://coco2-project.eu/structure)

2.2 Scope of this deliverable

2.2.1 Objectives of this deliverable

This deliverable aims to document the *in situ* and ancillary data requirements across the CoCO2 project, from WP2 through WP6. The documentation of these data needs is critical in order to move the work from a scientific exercise to an operational capacity. Through the documentation of these needs, the dependencies will become clear and potential weak links in the provision of timely emissions estimates can be identified.

To this end, the data standards (e.g. methodologies, accuracy) and specifications (e.g. spatiotemporal resolution) for measurements and auxiliary information should be collected and described. This report builds upon the previous Deliverable 7.1, based on responses collected within the first year of the project, and will be followed by Deliverable 7.3 in month 36. The overarching goal is to provide guidance for programmatic decisions regarding *in situ* measurement networks and ancillary measurements.

The first iteration of this deliverable served as a basis for the identification of data providers in Task 7.2, which resulted in Deliverable 7.4. Likewise, this second iteration will inform the next generation of this document in Deliverable 7.5. Together these documents provide guidance for the development of the prototype of the operational data pipeline in Task 7.4, resulting in Deliverable 7.8.

2.2.2 Work performed in this deliverable

In the first year of the project, information was collected via an online survey, and this formed the basis of the first iteration of this document. (A detailed description of the survey design and testing is included in Deliverable 7.1.)

The survey was split into two main sections, one focussing on *in situ* measurements, and one on ancillary and auxiliary data. Metadata about the respondent and their role in the project was collected in a separate introductory segment. The sections that were included are listed in Table 1. If a respondent indicated that he or she made use of data from a given category, they were directed to follow-up questions about how they were using the data, as well as their requirements for the data, namely: the pre-processing, measurement precision, spatial distribution, access, and timeliness. The full survey is still available to view (and even complete) here.

Feedback from respondents to the online survey indicated that it was not always clear what level of detail was desired in the response. Furthermore, it was unclear if the responses should reflect what data they were currently using, or rather what they would generally consider valuable.

To make the data collection more efficient, and reduce the uncertainty of the respondents, we decided to carry out interviews in the second year of the project, separated by work package. Notes were taken during the interviews in an online document by two colleagues simultaneously, allowing for a third to lead the discussion. The information collected and the categories considered were essentially the same, but collecting the information from several participants in parallel led to informative discussions. The interviews took place from April through July, and included 10-16 participants (including the interview team, who were also sometimes simultaneously respondents).

The information presented here represents a compilation of the responses from the first and second years of the projects. The *in situ* data needs are described in Section 3, while the ancillary and auxiliary data needs are documented in Section 4.

Table 1: List of the data streams that were included in the surveys, both online and through interviews.

In situ data needs	
Q1	Eddy covariance flux data
Q2	*In situ* CO$_2$ measurements
Q3	*In situ* CH$_4$ measurements
Q4	*In situ* measurements of co-emitted species
Q5	Measurements from urban networks
Q6	Ocean fluxes/partial pressures
Q7	Radiocarbon
Q8	Other tracers (e.g. radon, OCS)
Q9	Ground-based remote sensing (e.g. TCCON)
Q10	Site-level ecosystem parameters
Q11	Site-level information on management and/or lateral fluxes
Q12	*In situ* soil moisture
Q13	*In situ* meteorological measurements
Q14	Anything else?
Ancillary/auxiliary data needs	
Q1	Meteorological fields
Q2	Nightlights
Q3	Activity data
Q4	Satellite-based indices
Q5	Satellite-based measurements of SIF
Q6	Other satellite-based measurements
Q7	Landcover maps
Q8	Concentration fields from a global model
Q9	Anything else?

2.2.3 Deviations and counter measures

No significant deviations arose and no countermeasures were undertaken. Because we found it difficult to get sufficient feedback to the online survey, we implemented (online) interviews for the data collection in the second year of the project. This resulted in feedback from more participants, and should provide a more complete picture of the *in situ* data needs within the project.

3 *In situ* data needs

The first part of the survey focussed on the use of *in situ* measurements throughout the project. The responses for each type of data are summarized below. For each data type there is a summary of which work packages and tasks were making use of the data, and to what end. The timeliness needs of the data users is explicitly described, as this information is particularly important for the design of the operational data pipeline.

3.1 Eddy covariance flux data

Eddy covariance flux tower data were being used by respondents from WPs 2 through 5. Of these, the most intense users were working on biospheric flux modelling, particularly in WP2 and WP3. When considering this data stream, we distinguished which specific measurements were used: only CO$_2$ flux measurements, or also moisture and energy fluxes? Was the direct measurement of net CO$_2$ fluxes used (NEE, or net ecosystem exchange), or rather the model-derived partitioning into gross primary production (GPP) and ecosystem respiration? Flux tower data typically contain by gaps due to instrument problems and meteorological conditions under which the technique does not work well, e.g. stability. Consequently, gap-filled data sets are often used rather than raw measurements; the survey attempted to capture this use of processed vs raw data.

3.1.1 Near-real-time data needs

At the time of the data collection, only Task 3.1 had indicated that near-real-time eddy covariance flux data were needed. This task, which makes use of fluxes of CO$_2$, energy, and moisture as well as site-level meteorology, focusses on the evaluation of modelling and data assimilation developments in the global CO$_2$ MVS. Quality-controlled, gap-filled data are needed, with partitioning of the measured CO$_2$ fluxes into GPP and ecosystem respiration. The sigma values given by the data providers were used to estimate the measurement uncertainty. Data from all stations were considered, as they are working on a global scale. For evaluation purposes, data at different time scales are used (e.g. hourly, daily, weekly), depending on which scale of flux variability (diurnal, synoptic, seasonal) is being evaluated. For near-real-time data, the ICOS Carbon Portal was listed as a current source of measurements, although the standard data product there is released only annually.

The biggest concern with the use of the measurements was unreliable data quality (e.g. negative values for GPP), limited global coverage, and temporal delays. Temporal delays are related largely to the delayed data releases, as described in the following paragraph. A lack of stations particularly in the Tropics was identified, as well as potential biases towards undisturbed sites in site selection. The correction for storage flux was considered particularly challenging for some sites, leading to datasets that are difficult to compare to one another.

It should be mentioned that additional users (e.g. for prior biospheric flux products related to WP2) indicated that they foresee the need for near-real-time flux tower data in the future, as their products become operationalized, but are presently using data with approximately a year delay, or as they become available. The team producing FLUXCOM described receiving data through direct contact with FLUXNET colleagues, but indicated that they were ready to use routine data releases through ICOS. It was indicated that the Australian and US programmes are likely moving to annual data releases soon, and that ICOS was exploring data releases three times a year, rather than the current annual data releases.

The FLUXCOM team further indicated that they currently employed their own automated quality control tools to screen the data, rather than (and/or in addition to) using the quality-controlled data provided by FLUXNET.

3.1.2 Needed for use in year of simulation

One respondent taking part in Task 4.4 (national-scale inversions) indicated in the first year of the survey that they would be using flux measurements from the simulation year directly. However, further discussion indicated that this was rather for the purpose of evaluating the modelled fluxes rather than direct assimilation, and as such is documented in the following sub-section.

3.1.3 Needed only afterwards for model evaluation

One of the national-scale flux inversion modelling groups from Task 4.4 indicated that they would be using quality-controlled total CO$_2$ flux measurements to evaluate the NEE fluxes in their model. All stations within their (regional) modelling domain were considered for this purpose at a temporal resolution of one hour, potentially aggregating in time after sampling to model to ensure consistency in the approach. At present, this group was getting the measurements directly from the station PIs.

Two respondents from WP5 indicated that they are using eddy covariance flux data for model evaluation, specifically within Task 5.2, which focusses on site-level simulations of land surface models, and Task 5.6, which assesses inverse modelling results. While Task 5.6 was only using CO$_2$ flux measurements (quality-controlled, gap-filled, partitioned into GPP and ecosystem respiration), Task 5.2 was also considering using energy and moisture fluxes in addition to CO$_2$ fluxes (quality-controlled and partitioned, but without gap filling). Both groups used the quality flags provided with the data, and were using the data at half-hourly or hourly resolution (as well as aggregated scales). The respondent from Task 5.2 mentioned concerns about the quality of the data that were readily available, and as such preferred to use only data from stations that they knew to be reliable. Issues related to Intellectual Property Rights when using others' data were also mentioned as a concern. In contrast, the respondent from Task 5.6 was happy to make use of all data available, and was currently accessing data through ICOS and/or FLUXNET. They considered the representativity of the available datasets to be the biggest concern.

In the first year of the study, a respondent from Task 3.2 reported that the use of urban flux tower measurements was planned, for the evaluation of anthropogenic emission inventories from WP2. To this end, the use of raw flux measurements from urban and residential sites was foreseen at temporal resolutions as high as that of the model timestep (10 to 20 minutes, though hourly or 3-hourly data were preferred). This work has progressed in the second year of the project, with WP3 making use of urban flux tower data directly from providers in WP7. At present the use is largely for the purpose of model evaluation, without stringent timeliness requirements.

Furthermore, Task 3.3 will be using CO$_2$, moisture and energy fluxes (quality-controlled, gap-filled, partitioned data) in order to evaluate improvements in land use/land cover and prognostic leaf area index (LAI) mapping. In this case, the use of all sites is foreseen, addressing a range of temporal scales, from diurnal to seasonal to interannual. Data access is expected to be through ICOS and FLUXNET.

3.1.4 Data from other years can be used

Several respondents indicated that they were using measurements from eddy covariance flux towers for the purpose of parameter estimation, such that measurements from previous years could be used. (This usage was sometimes in addition to other timeliness needs, as in Tasks

3.1, 3.2 and 3.3 – more than one answer was possible per response.) Flux tower data was used for parameter estimation in Tasks 2.1, 3.1, 3.2, and 3.3, and in the Simple Diagnostic Biosphere Model (SDBM) that forms part of the Carbon Cycle/Fossil Fuel Data Assimilation System (CC/FFDAS) system used in WP3 and WP5.

In Task 2.1, the gap-filled, quality-controlled partitioned CO$_2$ flux measurements from sites representative of certain land cover types are used to estimate model parameters in the diagnostic vegetation model VPRM (Vegetation, Photosynthesis and Respiration Model). In this case, sites from the domain of interest (Europe) are used from other years, relying on the half-hourly fluxes from the FLUXNET 2015 release. The main concern was that some land cover types are poorly covered (e.g. semi-arid regions of the Iberian Peninsula), but a lack of coverage was a major issue in the Tropics. Similarly, the SDBM used within the CC/FFDAS makes use of eddy covariance flux data from other years to calibrate the model parameters.

The responses from Tasks 3.1 and 3.2 are discussed in more detail above in Section 3.1.1 and 3.1.3, respectively. In addition to these near-real-time and evaluation applications, these tasks are employing (or will be employing) flux measurements for parameter estimation as well.

There were two responses from Task 3.3 in the first round of the survey, one of whom is also described in more detail in Section 3.1.3. Both of these respondents are working on updates and improvements to vegetation and land cover modelling (one specifying that this is in CHTESSEL), and the impact that these changes have on the biogenic fluxes. Here, hourly measurements of carbon, energy, and moisture fluxes were employed, using quality-controlled data and partitioned carbon fluxes. The uncertainties provided with the data were not considered. Currently the data were accessed from FLUXNET and/or ICOS. Concerns about the data included the format, quality, and the limited coverage of the measurements.

3.2 *In situ* atmospheric mixing ratios of CO$_2$

Regional-scale modellers in WP4 were the primary users of *in situ* measurements of the atmospheric mixing ratio of CO$_2$. Of these, almost all (9 from 10) were making use of quality-controlled measurements while one group reported using raw measurements. While these data found the most use in WP4, which is focussed on regional-scale simulations, from plumes to national-scale inversions, the data were also used in WP5 (for the evaluation of inversion results) and WP3.

3.2.1 Near-real-time data needs

This response remains unchanged from the first round of the survey. Only Task 3.1 has reported needing these data in near-real-time up to now, for the time-sensitive evaluation of the modelling and data assimilation developments in the global CO2MVS at ECMWF. In this case, quality-controlled measurements are needed, and the measurement uncertainty provided with the data is considered. Hourly data are used, taking advantage of data from all available sites. At present these data are provided in near-real-time from the ICOS Atmospheric Thematic Centre (ICOS-ATC), and with delay from NOAA's ObsPack. The biggest concerns with the use of these data are the limited coverage and temporal delays, although these delays (particularly with ObsPack) have decreased in recent years as the demand for timely data has increased. The sparsity of measurements in the tropics is seen as a major limitation for global data coverage.

3.2.2 Needed for use in year of simulation

In particular, the national-scale inversions of Task 4.4 and the city-scale inversions of Task 4.3 reported needing *in situ* measurements of atmospheric CO$_2$ mixing ratios for direct assimilation. All but one reported using measurement uncertainties (precision/accuracy) that were reported with the product when assimilating these. These responses largely overlap with the regional-scale inversions that are contributing to WP5. Most users reported making use of all measurements available within their domain, with only one reporting a selection based on how well the model can represent a given measurement site. Data were generally assimilated at either native temporal resolution or at hourly resolution.

One data user remarked that the estimated model-data mismatch was so much larger than the estimated measurement uncertainty of the highly-precise measurements typical of ICOS and similar networks compliant with the WMO guidelines (e.g. NOAA, CSIRO, ECCC), that the reported uncertainties could largely be neglected. This may be different with the urban measurement networks currently being implemented e.g. in the ICOS Cities project. For the example of Zurich, the measurement uncertainties on in situ measurements of atmospheric CO_2 are closer to 1 ppm, but the gradients are so much larger in this context that the requirements are different.

The access to these data with the timeliness required seems to be a limiting factor. Some reported various efforts to gather databases, such as the ICOS 2018 drought task force (which fast-tracked the availability of some measurements within Europe) or the accelerated ObsPack releases. ICOS was named as their main access to European measurements by five respondents, and NOAA/ObsPack, the World Data Centre for Greenhouse Gases (WDCGG) and direct contact to measurement PIs were also mentioned. Specific mention was made of measurements from the UK and from stations operated by the Max Planck Institute for Biogeochemistry, which are not currently distributed through ICOS or other operationalized channels. The lack of availability of data from the Cabauw station in the Netherlands was highlighted by one respondent in the interviews in 2022. One user, simulating Krakow within Task 4.3, mentioned specific non-public data that are being collected within CoCO2, and potential issues related to the inhomogeneity of the timing of the campaign days. General concerns listed by the data users were limited coverage and temporal delays. With respect to coverage, the Iberian Peninsula was mentioned explicitly as a region in Europe with few measurements. Globally, there are many other gaps, particularly in the Tropics.

3.2.3 Needed only afterwards for model evaluation

Task 5.6 reported using *in situ* measurements of atmospheric mixing ratios of CO_2 for evaluation purposes. For this application they are using all the quality-controlled data they can find at the native temporal resolution, taking the measurement uncertainty into account. These datasets were being sourced from ICOS, NOAA, and WDCGG.

There were also two respondents from Task 4.1 who were using *in situ* measurements of CO_2 to evaluate plume simulations carried out by different models. The answers corresponded to two of the cases that will be simulated, namely the Randstad region of the Netherlands and Paris. For these cases specific *in situ* measurements were considered, including urban and peri-urban measurements. It was also the only explicit mention of aircraft-based measurements, though this may have been implicit in the other responses. As before, quality-controlled data are used, with temporal resolution up to minutes considered (where available) for these high-resolution simulations. Unlike the other users of this data stream, these respondents were more reliant on local PIs rather than operational data centres, reflecting the plume-scale focus of the simulations. Concerns listed were the heterogeneity of the available measurements and poorly quantified uncertainties.

One respondent from Task 4.4 also explicitly mentioned using *in situ* measurements of CO_2 to evaluate the national-scale inversion, presumably through comparison of optimized concentrations to *in situ* measurements that were not assimilated.

Campaign-based data were highlighted by respondents in the WP5 interview as being useful for model evaluation. It can be difficult for users to find these data at times, the activities of the ATMOS-ACCESS project (https://www.atmo-access.eu/) were highlighted as a potential solution to this problem.

3.2.4 Data from other years can be used

One of the respondents from Task 4.1 also identified that the plume simulations in this task would be used for parameter estimation, to help optimize model settings for simulations at these high spatial scales. All other aspects of their response are captured in the description in Section 3.2.3. One respondent from Task 4.4 also described the use of these measurements from other years to determine optimal model settings.

3.3 *In situ* atmospheric mixing ratios of CH_4

The respondents who reported using in situ measurements of atmospheric mixing ratios of methane (CH_4) are to a large degree a subset of the people who reported using *in situ* measurements of atmospheric CO_2, described in Section 3.2. As such, many of the answers overlap as a result. Of these, all but one were making use of quality-controlled measurements (seven of eight of online respondents) while one reported using raw measurements. These data are used widely in WP4 inversions on national and city scale (Tasks 4.4 and 4.3, respectively). Besides WP4, the data are also applied in WP5 (for the evaluation of inversion results) and in WP3.

3.3.1 Near-real-time data needs

As for CO_2, only Task 3.1 reported needing these data in near-real-time for the evaluation of the modelling and data assimilation developments in the global CO2MVS at ECMWF. For a more complete description of this data use, refer to Section 3.2.1.

3.3.2 Needed for use in year of simulation

The direct use of these measurements through assimilation was dominated by WP4, specifically Tasks 4.3 and 4.4. Most of the responses are similar to those for CO_2, found in Section 3.2.2. There were some differences in terms of access to the data: one user mentioned that they relied upon project-specific efforts to gather datasets (e.g. in VERIFY), while another mentioned that some sites were still not reporting data as long as two years after the measurements were collected.

3.3.3 Needed only afterwards for model evaluation

As previously described for CO_2 in Section 3.2.3, Task 5.6 is using *in situ* measurements of atmospheric mixing ratios of methane for the purpose of evaluating inverse modelling results. For this application they are using all the quality-controlled data they can find at the native temporal resolution, taking the measurement uncertainty into account. These datasets were being sourced from ICOS, NOAA, and WDCGG.

One respondent from Task 4.4 also explicitly mentioned using *in situ* measurements of methane to evaluate their national-scale inversion results, through the comparison of optimized concentrations to *in situ* measurements that were not assimilated.

3.3.4 Data from other years can be used

As in Section 3.2.4 for CO_2, one respondent from Task 4.4 described the use of *in situ* methane measurements from other years to determine optimal model settings.

3.4 *In situ* atmospheric mixing ratios of co-emitted species

In the first, online version of the survey, five respondents from WP3 and WP4 reported making use of *in situ* measurements of co-emitted species. In all cases, CO and NO_x/NO_2 were named as the species of interest, and in all cases quality-controlled data were used.

3.4.1 Near-real-time data needs

Only Task 3.1 indicated a need for these measurements in near-real-time, in parallel to the responses regarding *in situ* measurements of atmospheric CO_2 and CH_4. Here all available data were used at hourly spatial resolution, and currently data were being sourced from ICOS-ATC and air quality networks. Measurement uncertainty provided by the data providers was used. Limited coverage and temporal delays were identified as limiting factors in the use of these measurements.

3.4.2 Needed for use in year of simulation

Within WP4, two of the inversion teams were working on multi-species inversions, using co-emitted tracers including CO and NO_2. While the *in situ* data were used to some degree, there was a greater emphasis on the use of satellite measurements of these species.

3.4.3 Needed only afterwards for model evaluation

The non-operational work in Tasks 4.1 and 4.2 make use of measurements of co-emitted tracers to assess model simulations of plumes. However, most of these comparisons were primarily reliant on satellite measurements, or flight campaign data. When *in situ* measurements of co-emitted species were used, the measurements were sourced from the EEA, air quality databases, or local sources, with CO from ICOS and ICOS-like GHG measurement sites being used. Two respondents from Task 4.4 reported using only data from sites representing regional rather than local signals, such as rural background sites. One of the respondents from Task 4.1 preferred using measurements when CO_2 was co-sampled, but would use everything for evaluation purposes. Temporal scales from minutes to hours were used. One user reported that for air quality data, the formats are not always consistent. Harmonizing the format would save time. Data from other years can be used

One of the respondents from Task 4.1 (plume simulations) expressed that data from other years could be used, as they were focussing on optimizing chemistry and transport settings.

3.5 Measurements from urban air quality networks

The responses for this section were not updated based on the interviews conducted in the second year of the project, and the responses from the previous year were considered still valid. Three respondents reported making use of measurements from urban air quality networks, specifically in Task 3.2 (for evaluating anthropogenic emission inventories) and Task 4.1 (plume modelling). Within Task 4.1, atmospheric abundances of CO_2, CO, NO_2, NO, and (for one respondent) ozone were of interest, and quality-controlled data were used. Temporal resolutions from minutes to hours were found to be useful, and any measurements within the regional domain of interest (specifically Rotterdam, Amsterdam, Paris, Berlin, or at stack level) were sought. The data were being sourced through station PIs, national organisations, air quality databases, or through colleagues. One concern with the available data was the lack of co-located meteorological measurements.

In Task 3.2, the interest was in raw urban flux measurements of CO_2 (and NO_x, if available) and any meteorological measurements. In theory, all data were welcome at a temporal resolution ranging from tens of minutes to hours, but these measurements had not yet been accessed.

3.5.1 Near-real-time data needs

No users expressed a need for urban air quality networks in near-real time.

3.5.2 Needed for use in year of simulation

Task 3.2 expressed the need for these (flux) measurements specific to the year being simulated.

3.5.3 Needed only afterwards for model evaluation

All three respondents indicated that these measurements would be used for evaluation purposes, and thus would still be of use with some temporal delay. (The quantitative representation of air quality tracers within urban environments is quite challenging, but a qualitative comparison and evaluation could still be useful.)

3.5.4 Data from other years can be used

One of the respondents from Task 4.1 and the respondent from Task 3.2 indicated that data from other (previous) years could still also be used for e.g. parameter estimation or optimization of model chemistry.

3.6 Ocean fluxes/partial pressures

During the first year of the project, only one user from Task 4.4 indicated an interest in using ocean flux measurements in national-scale inversions. At this point the potential use was rather exploratory in nature, but they were considering using quality-controlled measurements for areas near Europe. The data were not in use yet, but an application of these measurements for parameter estimation, model evaluation, and direct assimilation were all being considered.

During the second year of the project, ocean partial pressure measurements were assimilated into an ocean model to create a flux product within Task 2.1 that was distributed within the project via ftp.

3.6.1 Near-real-time data needs

No near-real-time data needs were reported for measurements of ocean fluxes or partial pressures.

3.6.2 Needed for use in year of simulation

The respondent from Task 4.4 indicated that direct assimilation of ocean flux and/or partial pressure measurements from the year of simulation was being considered in an exploratory manner.

3.6.3 Needed only afterwards for model evaluation

The respondent from Task 4.4 reported that measurements of ocean flux and/or partial pressure might be used for model evaluation.

3.6.4 Data from other years can be used

Depending on what comes of the exploratory use of these measurements, the respondent from Task 4.4 considered that these measurements might be used for parameter estimation.

3.7 Radiocarbon in CO$_2$

Respondents from both WP4 (Tasks 4.3 and 4.4) and WP5 indicated that they planned to use measurements of radiocarbon in CO$_2$ for the purpose of source attribution. Both users wanted to make use of quality-controlled measurements, and would make use of measurement uncertainty if available. All measurements within the domain of interest (Europe for Task 4.4 and/or Krakow in the case of Task 4.3) were being considered. For use within the global CC/FFDAS system in WP5, measurements from stations around the world would be used.

Because radiocarbon measurements are sometimes integrated over a longer measurement period (e.g. two weeks at ICOS Class 1 stations) and sometimes are instantaneous, as in campaign-based flask measurements, both temporal scales need to be considered. Both users indicated that they would use both types of measurements, based on availability.

Regarding the source of the measurements, for the Krakow domain the campaign data from WP7 is being exploited, in addition to data provided directly from station PIs and ICOS. The other respondent indicated using ICOS and NOAA measurements, or contacting data providers directly. All respondents indicated the availability of these measurements was the most important limitation at present, both spatially and in terms of temporal coverage. It was hoped that the coming Horizon Europe project CORSO (CO2MVS Research on Supplementary Observations), which is developing a database of radiocarbon measurements, might help improve the data limitation problem in the future.

3.7.1 Near-real-time data needs

No users reported a need for near-real-time measurements of radiocarbon at this point.

3.7.2 Needed for use in year of simulation

All respondents indicated that they planned to directly assimilate the measurements in their activities, and as such required measurements from the year of simulation.

3.7.3 Needed only afterwards for model evaluation

Radiocarbon measurements were not identified for use in model evaluation.

3.7.4 Data from other years can be used

No users reported using radiocarbon measurements from other years, e.g. for parameter estimation.

3.8 Atmospheric mixing ratios of other species

This question was included to assess the use of additional tracers such as radon, carbonyl sulphide, or atmospheric potential oxygen.

Respondents from WPs 3, 4, and 5 reported using radon measurements, as available. All users indicated that they wanted quality-controlled data from as many sites as possible, with temporal resolution from minutes to hours. The goal is primarily to assess representation of the planetary boundary layer height in transport models. Currently, three of the respondents indicated that they accessed these data directly from the station PIs, through personal contacts, or through national networks (in one case). Only one respondent indicated accessing these data through ICOS-ATC, and this was for near-real-time application. All users reported that the limited coverage of these measurements was the most serious limitation to their use.

The use of carbonyl sulphide was also mentioned, but is not being pursued actively within CoCO2 with the goal of operationalisation.

3.8.1 Near-real-time data needs

Task 3.1 was the only task in the project which identified the near-real-time application of radon measurements. In this case, data access through ICOS-ATC was reported.

3.8.2 Needed for use in year of simulation

No users reported assimilating these data directly for the year in question, but in a non-near-real-time capacity.

3.8.3 Needed only afterwards for model evaluation

Respondents from Task 4.1 (plume simulations), Task 4.4 (national-scale inversions) and Task 5.6 (evaluation of inverse modelling results) reported using these data for evaluation purposes, for which a delayed delivery was not critical.

3.8.4 Data from other years can be used

Respondents from Task 4.1 reported that data from other (previous) years could also be used, e.g. for parameter estimation or model optimization.

3.9 Ground-based remote sensing measurements of atmospheric composition

Respondents from across WPs 3, 4, and 5 reported using or planning to use ground-based remote sensing measurements of atmospheric trace gases within the project. All planned on making use of XCO_2 (total column atmospheric CO_2) measurements, four planned on using XCH_4 measurements as well, and one reported using column-integrated carbon monoxide measurements (XCO) in addition to the other two species. Most reported using data from the TCCON network, some also reported using data from COCCON sites.

3.9.1 Near-real-time data needs

Task 3.1 indicated needing XCO_2, XCH_4, and XCO measurements in near-real time in order to evaluate the modelling and data assimilation developments in the global CO2MVS. For this purpose, hourly data were sufficient, and were currently accessed them directly from the TCCON database, taking the reported measurement precision into account while using them. Both limited coverage and temporal delays were identified by this respondent as significant limitations in the use of this data stream.

3.9.2 Needed for use in year of simulation

No users reported using these data for direct assimilation in (non-IFS) simulations.

3.9.3 Needed only afterwards for model evaluation

The respondents from WPs 4 and 5 indicated that the measurements were used primarily for evaluation purposes, and as such a delay in their availability is less critical. This included one respondent from Task 3.2 (implementing and evaluating anthropogenic emission inventories), two from Task 4.1 (plume simulations), two from Task 4.4 (national-scale inversions), and one from Task 5.6 (evaluation of inverse model results). Most of these users reported accessing the measurements through the TCCON data archive. Within Task 4.1 (a scientific, non-operational activity), station PIs were contacted directly in order to access EM27 measurements that are not part of TCCON. COCCON measurements were also used, for XCH_4 and XCO_2. Two respondents indicated that limited data coverage in some areas was a shortcoming of this data stream.

3.9.4 Data from other years can be used

No respondents indicated that ground-based remote sensing data from other years could be used for their activities within the project.

3.10 Measurements of site-level ecosystem parameters

Within Task 5.2 it was reported in both years of the project that site-level measurements of ecosystem parameters, specifically leaf area index (LAI), could be useful for their site-level simulations. In one case, they were be using quality-controlled measurements on daily to monthly temporal resolution, specifically for the flux tower site in Toulouse. Sampling time was considered to be the most critical issue with this data stream.

On a more systematic level, respondents from Task 5.2 indicated that such data would be particularly useful if they would be more readily available from many stations. This lack of comparable, widespread data is the primary reason why such measurements are not currently being incorporated into upscaling approached. Such data sare more readily available from

ICOS stations, and a need for a coordinated approach with other (eddy covariance flux tower) sites and networks to standardize such data collection was identified. This was taken as an action in meetings planned across networks in September, 2022, in order to identify which ecosystem parameters should be prioritized for collection.

3.10.1 Near-real-time data needs

No near-real-time need for this data stream was reported within the project.

3.10.2 Needed for use in year of simulation

No respondents reported directly assimilating site-level measurements of ecosystem parameters.

3.10.3 Needed only afterwards for model evaluation

The respondent indicated that these data would be used for model evaluation purposes, and a temporal delay was not critical.

3.10.4 Data from other years can be used

No use of site-level measurements of ecosystem parameters for parameter estimation was reported.

3.11 Information about site-level management and/or lateral fluxes

No respondents indicated that they were currently utilizing site-level information about management (e.g. ploughing, harvest, fertilizer) or related lateral fluxes (e.g. wood harvest in forests, organic manure in crop fields and grasslands).

Despite this, data about management was identified by several users across multiple tasks in WP2, WP5, and WP7 as being of critical importance. To some degree, this overlaps with the previous category, as having site-specific high-quality data related to e.g. crop harvest and fertilisation would be the first step in being able to use such information to improve biospheric flux priors. Scaling this up would require information on a global level (potentially through remote sensing), but having usable site-level information is a necessary first step.

Within WPs 3 and 4, a lateral flux product produced outside the project by project participants is being tested. This is already an elaborated product, rather than direct measurements of the lateral fluxes. Because this product is not being produced within CoCO2, its data requirements are not considered in this report.

3.12 *In situ* soil moisture measurements

No respondents reported using *in situ* measurements of soil moisture within this task. Within Task 2.1 the team behind FLUXCOM reported looking at soil moisture measurements when they were collocated with flux towers. One respondent from WP5 mentioned that it would be beneficial to consider soil moisture measurements when using atmospheric radon measurements to assess transport, but was not yet using such measurements.

3.13 *In situ* measurements of meteorological parameters

Users from across WPs 2, 3, 4, and 5 reported directly using *in situ* measurements of meteorological parameters. This was done on different scales. Within WP2 and the biospheric flux assessment activity of Task 5.6, site-level meteorological data are considered particularly important. Most users reported using quality-controlled measurements, though individual users from Tasks 4.3 and 4.4 reported using both raw and quality-controlled data.

3.13.1 Near-real-time data needs

None of the respondents reported needing *in situ* meteorological measurements in near-real time at this point, beyond their already operational use in the IFS.

3.13.2 Needed for use in year of simulation

The respondent from Task 3.2 indicated that meteorological measurements from the current year would be needed for the implementation and evaluation of anthropogenic emission inventories. For this task, only urban measurements of relevant NWP variables (e.g. 2-m temperature, 10-m wind speed) would be used, with a temporal resolution ranging from model timestep (10-20 minutes) to 3-hourly. These data were not yet actively being used.

One respondent from Task 4.3 (city-scale inversions) and one from Task 4.4 (national-scale inversions) reported directly assimilating *in situ* measurements of wind speed and direction within their modelling domain. For this, a temporal resolution of hourly (or native) was foreseen. For the national-scale inversions the user reported retrieving the data from the ICOS Carbon Portal, and found that mast corrections and data availability to be the most challenging aspects related to its use. Other users within Task 4.4 indicated interest in potentially directly assimilating meteorological measurements along with greenhouse gas atmospheric mixing rations, but this was largely seen as an experimental plan at this point.

One group within Task 4.2 had planned to directly use *in situ* meteorological measurements in their convolutional neural network approach to plume inversion, but found no benefit from their inclusion up to this point. As such, they will rather be using the data for model evaluation instead.

3.13.3 Needed only afterwards for model evaluation

In Task 5.6, direct measurements of planetary boundary layer height are being used for the purpose of model evaluation. In this case, the data are being collected directly from station PIs and applied at native temporal resolution. The most limiting aspect of this data stream is reported to be the correct application of the measurement uncertainties.

Within Task 4.1, *in situ* measurements of wind and temperature were used for model evaluation of the plume simulations, with some additional use of moisture, boundary layer height, surface heat flux, moisture flux, and ground heat flux measurements. All available measurements with temporal resolutions from minutes to hourly within the domain of interest were considered. The data were obtained from either national networks or meteorological databases. The lack of co-located meteorological and atmospheric composition measurements was named as a limiting factor in making optimal use of these data.

The respondent from Task 4.4 indicated that wind measurements were used for model evaluation as well, particularly to explore complicated transport features.

3.13.4 Data from other years can be used

A respondent from Task 2.1 reported on the use of *in situ* meteorological measurements from flux tower sites for the purpose of parameter estimation in the context of ecosystem modelling. In this case, incoming shortwave radiation and air temperature measured at eddy covariance flux tower sites representative of specific plant functional types were used. Half-hourly data were used, and the data were taken from the FLUXNET 2015 release.

The respondents from Task 3.2, 4.4 and one respondent from Task 4.1 (described in more detail in Sections 3.13.2 and 3.13.3) also characterized their use of *in situ* meteorological measurements in terms of parameter estimation or model optimization, for which measurements from other years could be used.

4 Ancillary/Auxiliary data needs

All survey respondents reported using at least some ancillary or auxiliary data in their activities within CoCO2. Their data needs are reported here, following a similar format to that for *in situ* measurements in Section 3.

4.1 Meteorological model fields

Almost all respondents reported using fields from meteorological models within their activities in the project, from WPs 2 through 5. Different products were used, mostly from ECMWF (ERA5 or short-term forecasts) but also fields from Meteo-France were used. Respondents reported accessing meteorological fields through MARS, or ERA5 fields through the Climate Data Store (CDS) or local data pools (such as at the German supercomputing centre DKRZ). There were some concerns about the difficulty of access, with the CDS being somewhat slow when retrieving model-level fields (although this improved from 2021 to 2022). Retrieval with MARS was much faster and easier, though access is restricted and sometimes colleagues with full access have to be asked to retrieve data. (Users must apply to representatives of their national meteorological service, who regulate access to MARS. Depending on the country, this can be a limiting factor.) One user reported having to log in to ECMWF weekly to maintain access. One particular problem with timely access arose in 2022 with the migration of the ECMWF data centre to Bologna, during which access was restricted for some time. (This is not expected to be a recurring problem in the near future.)

Two respondents reported concerns about dealing with the data volume, and one commented that the GRIB1 and GRIB2 file formats were somewhat complicated to deal with. Only one user, from Task 3.2, reported using the IFS-ensemble to estimate uncertainties in the provided fields, though this was seen as an avenue worth exploring by respondents from WP4. The users were divided about the spatial resolution used, with approximately half reporting using ERA5 (at ~0.25° hourly resolution) and half reporting using short-term-forecast products with higher spatial resolution but 3-hourly temporal resolution. (One respondent reported using both.)

4.1.1 Near-real-time data needs

No users reported needing meteorological model fields in near-real time.

4.1.2 Needed for use in year of simulation

Most users reported needing these data for the year that they were simulating, including within Task 2.1 (for producing biospheric and ocean fluxes), Task 3.2 (for implementing and evaluating online anthropogenic flux models), WP4 (all tasks), and within Task 5.2 (site-level simulations).

4.1.3 Needed only afterwards for model evaluation

Both respondents from Task 3.3 indicated that they used meteorological fields for model evaluation after adapting their landcover schemes. Similar use was reported within Task 5.2 for the evaluation of site-level simulations. The respondents looking at plume-modelling case studies (Task 4.1) indicated that they were using the data for model evaluation as well, and as such had less stringent timeliness requirements.

4.1.4 Data from other years can be used

Feedback from Tasks 3.2, 3.3 and 5.2 reported the use of meteorological fields for model parameter estimation, for which data from other years could be used.

4.2 Nightlights

During the project's first year, one user reported using nightlight data to implement and evaluate online anthropogenic emission inventories within Task 3.2. However, this activity had not yet started in earnest, and as such, only rough information could be provided: using any available data at any resolution.

The CC/FFDAS system used in WPs 3 and 5 makes use of a nightlight product. No uncertainties are reported with the product, so some uncertainty is assumed by the users. The product used is based on VIIRS satellite data and distributed by the Colorado School of Mining on an annual basis. Previously a monthly product was available, which would be preferable, but this is no longer available

4.2.1 Near-real-time data needs

A near-real-time need for this data stream was not yet reported.

4.2.2 Needed for use in year of simulation

Within both the offline CC/FFDAS system and the online implementation of Task 3.2, the nightlight product is needed for the year currently being simulated. An annual product is currently being used, but a higher temporal resolution would be useful.

4.2.3 Needed only afterwards for model evaluation

No one reported needing these data *a posteriori* for model evaluation.

4.2.4 Data from other years can be used

The respondent from Task 3.2 also reported potentially using these data for parameter estimation, for which information from other years could be used.

4.3 Activity data

The primary use of activity data is in WP2, for the production of anthropogenic emission inventories. Classes of data used included fuel consumption data, population density maps, roads and traffic statistics, and residential heating. The CC/FFDAS system also uses gross domestic product (GDP) as a model input. Fuel consumption data are provided from the United Nations and IEA. Temporal resolution is currently yearly, but higher resolution would be useful. Open Street Map was being used for the distribution of roads, but traffic data was not yet being used in the CC/FFDAS approach.

Further user wishes included data aggregated on a sub-sectoral level, separating the activity based on the kind of combustion (e.g. coal, gas, etc.). When working on global products, some regions were more difficult in terms of the quality and completeness of the data, with Asia and Africa being mentioned in particular. Different sources of data were also sometimes difficult to combine, due to heterogenous formats and granularity.

Another difficulty in producing emission inventories is the exact location of point sources, such as power plants. Statistically, it is difficult to express the uncertainty in the location of a power plant, currently this was being done by one respondent from WP2 through adding uncertainty to pixel edges. Another source of uncertainty was related to the definition of the polygons for national boundaries, as the fuel use statistics are generally on a national level and have to be distributed within the area of the country.

Within WP3 activity data are also used for the purposes of evaluating anthropogenic emission inventories produced in WP2. Furthermore, it is common practice among respondents from WP4 to use annual fuel use statistics from British Petroleum (BP) to extend existing emission inventories to the following year, as the BP statistics are released before the elaborated emission grid maps.

4.3.1 Near-real-time data needs

No near-real-time data needs were reported, however, because the development of the emission inventories is reliant upon the provision of fuel use statistics that are generally released annually, having these statistics available on a higher temporal resolution (such as monthly) would allow for these emission inventories to be produced with less latency.

4.3.2 Needed for use in year of simulation

Data from the current year are needed for all categories of data discussed in this section.

4.3.3 Needed only afterwards for model evaluation

It was not reported that these data would be used for model evaluation or validation.

4.3.4 Data from other years can be used

The respondent reported that data from other years could presumably be used to evaluate the upscaling approach used in emission inventories.

4.4 Satellite-based indices

Satellite-based measurements of ecosystem properties, or at least the remotely-sensed spectrally-resolved reflectance data from which these are calculated, were used in WPs 2-5. MODIS reflectance data were used extensively for the production of the upscaled biospheric flux product FLUXCOM, as well as to drive the diagnostic biospheric model VPRM. FLUXCOM and offline VPRM fluxes are both produced in Task 2.1, and other users reported using VPRM online in their models in WP4. The fraction of absorbed photosynthetically-active radiation (FAPAR) is also derived from MODIS, and used as an input to the SDBM of the CC/FFDAS system, which is used in WPs 3 and 5.

Within WP2 and WP4, VPRM uses MODIS reflectance data to calculate EVI (enhanced vegetation index) and LSWI (land surface water index). In both cases they were using measurements with a spatial resolution from 500 m to 1 km at 8-day resolution, and accessed the data from a NASA ftp server. Both users were using the indices as input for the diagnostic biospheric flux model VPRM (Vegetation Photosynthesis Respiration Model, Mahadevan et al., 2008), one offline for the production of fluxes in Task 2.1 and one online as part of their regional-scale inversion framework in Task 4.4. One of the users identified the pre-processing of the data as a potential limitation, requiring poorly documented software with a remapping library that is no longer maintained. (This pre-processor is currently being rewritten in python to update the libraries and enable the use of additional satellite measurements once MODIS is discontinued in mid-2023.)

The team behind FLUXCOM (in Task 2.1) also reported a strong dependence on MODIS reflectance data, and reported that the use of these data created a lot of technical difficulties. For training the network, they need full-resolution cut-outs at flux tower sites globally. They also need the data globally for upscaling, but this can be done at a lower resolution. Currently they extract the data using Google Earth Engine for pragmatic reasons, but they are not entirely satisfied with this choice. It is easiest this way, but certainly does not conform to FAIR data practices, and only works as long as a private company continues to host such a service. The storage structure of the data is not optimal for performing time series analysis.

As MODIS will be decommissioned in 2023 (VIIRS Instruments Become More Essential As Terra and Aqua Drift from their Traditional Orbits | Earthdata (nasa.gov)), they are also looking into replacements, considering similar products from both NASA and ESA. In general, all teams working with MODIS report that they have found NASA data products easier to access than those from ESA. MODIS is still the backbone of their approach, but products from the Sentinels and VIIRS may provide an appropriate replacement. They are also considering passive microwave data as these provide additional information, but optical sensors have formed the foundation of their approach up to now.

Other respondents from WP3 reported using the Copernicus Global Land Service (CGLS) Leaf Area Index (LAI) product CGLS LAI v2, based on a daily synthesis of top-of-canopy (TOC) reflectance data from the PROBA-V satellite and the SPOT-VEGETATION Programme. This was for the purpose of improving land use and land cover mapping, prognostic LAI modelling, and evaluating the impact of land cover updates on the fluxes in CHTESSEL within Task 3.3. The data are used with a spatial resolution of 300 m and 1 km and with a temporal resolution from 3 to 10 days. The data were available through the CGLS and C3S portals. The most limiting factor in using the product was temporal delays.

4.4.1 Near-real-time data needs

No respondents reported needing these data in near-real time at present, although VPRM has been used in near-real-time for tracer forecasting in the context of a measurement campaign. A near-real-time 8-day reflectance product is available from MODIS.

4.4.2 Needed for use in year of simulation

All users reported needing the satellite-derived measurements for direct use in the year currently being simulated.

4.4.3 Needed only afterwards for model evaluation

One respondent from Task 3.3 reported that the data were also used for validation and evaluation purposes.

4.4.4 Data from other years can be used

The respondent from Task 3.3 also reported that data from other years could be used for testing and improving the land cover model.

4.5 Satellite measurements of SIF

During the first year of the project, Task 5.2 reported using spaceborne sun-induced fluorescence (SIF) measurements within the project, for the purpose of site-level simulations. Furthermore, it is used for comparison within this task, and in general by the FLUXCOM team for evaluation of their upscaled GPP product.

4.5.1 Near-real-time data needs

No near-real-time data needs were reported.

4.5.2 Needed for use in year of simulation

The data are needed for the year currently being simulated when used directly for site-level simulations, as reported by one modelling team.

4.5.3 Needed only afterwards for model evaluation

The use of these measurements for model evaluation (also within Task 5.2) can take place with a less stringent timeliness requirement.

4.5.4 Data from other years can be used

No users reported using these data for parameter estimation or similar within the project.

4.6 Other satellite-based measurements

Here, the question specified if other satellite-based measurements (other than atmospheric mixing ratios) were used. One user reported on their use of other satellite-based measurements of atmospheric composition nonetheless (GOSAT, IASI, OCO-2, GOME-2, TROPOMI), which is not included in the current report. One other user reported the use of LAI data, and this response has been included in Section 4.4, as it is, strictly speaking, a satellite-based index. Likewise, measurements of FAPAR based on MODIS reflectances are included in Section 4.4. Finally, one user reported general plans to use satellite measurements to characterize the land surface for plume simulations in Task 4.1, which is a non-operational exercise.

4.6.1 Near-real-time data needs

No near-real-time data needs were reported.

4.6.2 Needed for use in year of simulation

As the plume simulations are somewhat decoupled from the operational chain and are simulating scenes from the past, the data were not considered to be needed for the currently simulated year.

4.6.3 Needed only afterwards for model evaluation

The use of delayed data for model evaluation was foreseen.

4.6.4 Data from other years can be used

As the plume simulations focus on past years, this data use falls into this category.

4.7 Land cover maps

Many modelling groups responding to the survey and taking part in the interview reported using land cover maps within the project, from WPs 2 through 5. Different respondents interpreted this question slightly differently, but some general themes emerged. Respondents from Task 3.1, Task 3.3, Task 4.4, and Task 5.2 reported making use of the ESA-CCI land cover product. Three respondents from Task 4.4 described the built-in land surface schemes of their models (the static MODIS land cover map distributed with WRF, the static USGS land cover map distributed with WRF, and the multilayer land surface scheme TERRA of ICON). All of these are based on static maps that are based on data as much as 30 years old. Another respondent from WP4 reported using a landcover map that is distributed in ICON, which is fixed in time. (He was not sure which year it was fixed to.)

Similarly, one respondent from Task 4.1 reported in the online survey that a landcover map was used in their LES simulations, without further specification. One user from Task 2.1 reported using the SYNMAP product (Jung et al., 2006) but was planning to switch to the CGLS 100-m land cover map in the near future. One respondent from Task 5.2 reported using ECOCLIMAP in addition to the ESA-CCI product, and in Task 3.2, one of the users was using the ECMWF urban cover map from the Copernicus SLIM project.

Also from WP4, one user reported that the land cover map played a significant role for their simulation of CO$_2$. For one of their simulations, they tested two different land cover maps, resulting in significant differences.

The FLUXCOM team reported that they are using a land cover map, but wanted to move away from this approach. In addition to land cover types, they considered a mapping of C3 and C4 vegetation to be particularly important, but this is not currently available as an observation-based product, which is a problem. Instead they use inventories or a modelled distribution.

The spatial resolution required by users was often tied to the spatial resolution of the model used: in Task 3.3, users reported using the full 300-m resolution of the ESA-CCI product, in Task 5.2 resolutions from 300 m to 1 km were used. In Task 2.1, land cover maps are aggregated to the 1-km resolution of the flux product, taking into account the fractional land cover at higher resolution. The respondents carrying out national-scale inversions in Task 4.4 aggregated the land cover onto the resolution of their model, from 5 km to 13 km, and for the global IFS simulations in Task 3.1 the land cover map was aggregated to 9-km or 25-km resolution for forecast and analysis respectively. The urban cover map was used at 1-km resolution.

Temporally, the responses varied between those using essentially static maps (in Task 5.2, Task 4.4, Task 3.2 and currently for Task 2.1) and those who used annually updated fields (in Task 3.1 and 3.3).

The timeliness requirements for this data stream are somewhat different from most, as land cover maps tend to be updated either annually (or less frequently), or are essentially static in time. Two respondents (one from Task 3.3 and one from Task 3.1) indicated that they needed a landcover map specific to the year they were simulating. Several other respondents (from Task 2.1, Task 3.3, and Task 4.1) indicated that they were updating the landcover only when new products became available, but not regularly. Another group of respondents (from Task 3.2, Task 4.4, and Task 5.2) reported that they were using fixed maps, even when the data product might be available for later years, and the timeliness of the product was not critical.

Data users turned to different sources for accessing these maps, whether directly through the ESA landcover CCI website, in-house at ECMWF (for Task 3.2), through Meteo-France, the CDS, through DOIs linking to Zenodo, or C3S. The following factors limiting the use of these datasets were identified: limited temporal resolution (for reanalyses especially), uncertainties in converting land classes to model classes, temporal delays in the provision of the maps, and inflexible tools provided along with the datasets. One user commented that they themselves needed to be more proactive in regularly checking for updates. The comment was raised that it was easy to treat the land cover map as something of a “black box” in a NWP model when the code is distributed with a default product. This does not make it the best option.

4.8 Concentration fields from a global model

The regional modellers responding from WP4 reported that they were making use of concentration fields from a global simulation in their work within the project. In addition to feedback from WP4, there was one positive response from Task 3.1. As for the species needed, all but one respondent indicated that they were using CO_2 mixing ratio fields, and five indicated that they were using CH_4 mixing ratio fields. Five respondents were using some combination of co-emitted species, such as CO, NO_2, and other chemical tracers. Most were using products retrieved from ECMWF (via MARS) or CAMS, while one indicated that they calculate their own global model fields or use NOAA’s CarbonTracker product. One user from Task 4.1 indicated that they were using TROPOMI data for NO_2 and CO, which is not from a global model, but might provide lateral boundary conditions for plume modelling. The spatial resolutions used ranged from “the highest possible” to 3° x 2°, with temporal resolutions from hourly to 3-hourly. No users reported using uncertainties of any sort.

In the second year of the project, users mentioned that there was a reanalysis ensemble of tracers available at a lower resolution, which could provide some uncertainty in the background field, but that this was not yet part of the official CAMS distribution. In general, users reported that the documentation of the CAMS greenhouse gas tracer fields that are available was not particularly user friendly, and it was usually easier just to ask someone from ECMWF which product should be used for a given application. Furthermore, the CAMS forecast and analysis tracer fields are not available to all ECMWF accounts, so some users had to rely on colleagues downloading the fields on their behalf.

4.8.1 Near-real-time data needs

Only one survey respondent reported requiring these data in near-real time, for the evaluation of the modelling and data assimilation developments in the global CO2MVS within Task 3.1. Within this task, 3-hourly concentration fields at 9 to 30 km spatial resolution from the MARS archive were being used. The most limiting factor was found to be their temporal coverage.

4.8.2 Needed for use in year of simulation

All users but one from WP4 reported needing these data for the year actively being simulated, presumably as initial and lateral boundary conditions for regional simulations.

4.8.3 Needed only afterwards for model evaluation

One respondent from Task 4.1 reported using these data only for evaluation purposes, but also described using TROPOMI measurements for this purpose.

4.8.4 Data from other years can be used

No respondents reported use of this data stream from previous years.

5 Conclusion

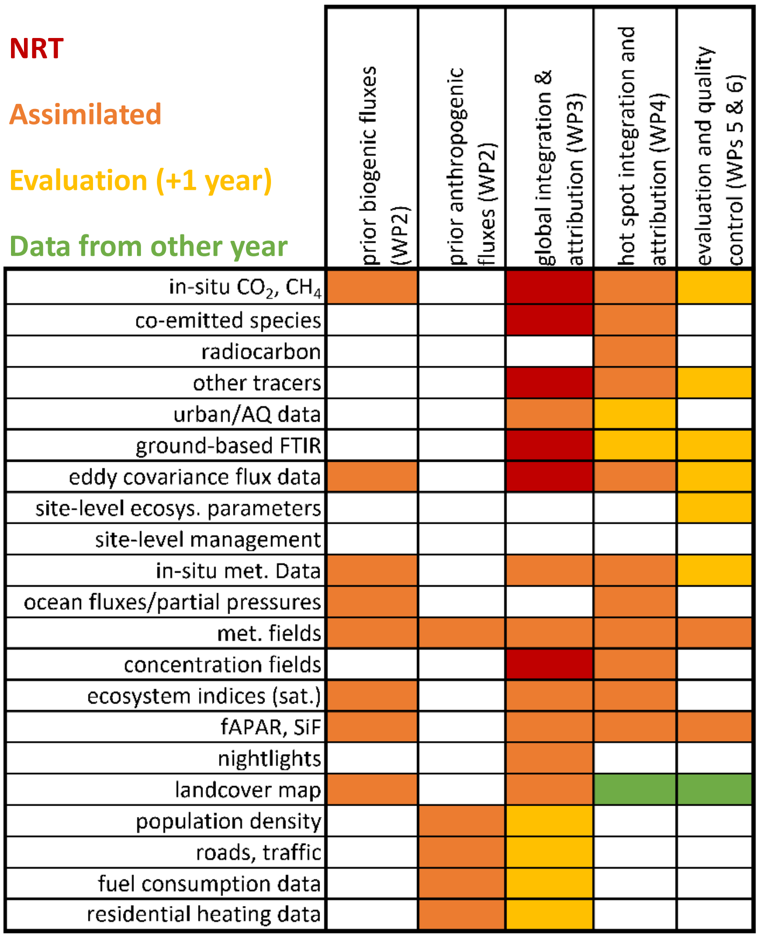
Based on the responses that were supplied, a picture of the data needs within the project has emerged. While it is clear that much of the data are needed in a timely manner, only the respondent from WP3 reported a need for near-real-time observations. This may, however, change over the remaining year of the project, as the prototype system shifts towards an operational implementation.

Rather than summarizing the results by project task, as was done in the first iteration of the report, instead the timeliness requirements are summarized by Work Package. This was chosen as it is thought to better represent the broader needs of the operational system, rather than being tied directly to the CoCO2 architecture. This may also make it easier for similar projects (e.g. on a national scale) to interpret the results in their context. Thus, results are now tabulated by overarching category, namely:

- Prior biogenic fluxes (WP2)
- Prior anthropogenic fluxes (WP2)
- Global integration and attribution (WP3)
- Hotspot integration and attribution (WP4)
- Evaluation and quality control (WPs 5 and 6)

The number of respondents per data category are no longer enumerated, to avoid ambiguities in double counting between the iterations of data collection. As in the initial version of the report, for each data type the most stringent reported timeliness requirement is colour-coded, with red representing near-real-time need, orange for use in the currently simulated year, yellow for use in model evaluation, and green for parameter estimation, for which other years of data could be used. Where no colour is shown, no respondents reported using this data stream in that part of the project. This visual summary is presented in Table 2.

Table 2: Summary of the timeliness requirements by broader task. The colours indicate the timeliness requirements of the different data streams by task, with red for near-real-time, orange for use in the currently simulated year, yellow for use in evaluation (for which a time delay of a year is considered acceptable), and green for cases where the measurements are used only for parameter estimation, and data from another year could be used. When more than one timeliness requirement was listed per task and data stream, the most stringent requirement is shown.



🟥 **NRT**

🟧 **Assimilated**

🟨 **Evaluation (+1 year)**

🟩 **Data from other year**

	prior biogenic fluxes (WP2)	prior anthropogenic fluxes (WP2)	global integration & attribution (WP3)	hot spot integration and attribution (WP4)	evaluation and quality control (WPs 5 & 6)
in-situ CO$_2$, CH$_4$	🟧		🟥	🟧	🟨
co-emitted species			🟥	🟧	
radiocarbon				🟧	
other tracers			🟥	🟧	🟨
urban/AQ data			🟧	🟨	
ground-based FTIR			🟥	🟨	🟨
eddy covariance flux data	🟧		🟥	🟧	🟨
site-level ecosys. parameters					🟨
site-level management					
in-situ met. Data	🟧		🟧	🟧	🟨
ocean fluxes/partial pressures	🟧			🟧	
met. fields	🟧	🟧	🟧	🟧	🟧
concentration fields			🟥	🟧	
ecosystem indices (sat.)	🟧		🟧	🟧	
fAPAR, SiF	🟧		🟧	🟧	🟧
nightlights			🟧		
landcover map	🟧		🟧	🟩	🟩
population density		🟧	🟨		
roads, traffic		🟧	🟨		
fuel consumption data		🟧	🟨		
residential heating data		🟧	🟨		

5.1 Dependencies and bottlenecks

As in the first edition of this report, it is clear that the near-real-time data needs of the project are largely driven by the global integration and attribution work in WP3, specifically the use of data within the IFS.

Obvious dependencies include the use of the global fields from WP3 as boundary conditions in WP4, especially as ensembles of modelling results from the regional scale systems should be included in the inversion system of the IFS. Here the use of boundary conditions from the CAMS GHG forecast branch may eventually provide a solution, or the additional information provided by the regional-scale modelling systems may only be included in a later reanalysis attempt.

Another dependency that may result in conflicts with timeliness requirements is the provision of prior fluxes, anthropogenic emission inventories in particular. Because the emission estimates can only be produced once the national-scale fuel use statistics are released, these will always lag behind the NRT data needs of WP3, which depends upon these emission inventories as a prior. A solution thus far has been to simply reuse the emission inventory for the previous year as a prior, perhaps adjusted based on e.g. temperature, assuming that the modelling system will be able to adjust accordingly, guided by the atmospheric measurements. This is a form of extrapolation, and should be approached with caution.

The timeliness requirements are not yet being met by many of the data streams that are needed in the project. Spaceborne measurements are clearly further ahead on this count, with satellite-derived indices, FAPAR, and SiF all meeting the current timeliness requirements. The upcoming retirement of MODIS creates some uncertainty for the indices and FAPAR measurements however, with groups actively testing the use of replacement products (like VIIRS, or the more highly-resolved Sentinel-2 data).

In situ measurements of carbon dioxide and methane are only partially compliant, with the NRT products produced by ICOS, and the operational airborne GHG measurements of IAGOS being examples of NRT *in situ* measurements. The ObsPack products compiled and released by NOAA are moving in this direction, with *in situ* atmospheric mixing ratio measurements of CO_2 now being released approximately quarterly (with more lag), and for methane approximately annually.

Some other data types exhibit a large degree of heterogeneity when it comes to the temporal availability of their measurements. An example of this is eddy covariance flux measurements. ICOS provides these ecosystem measurements on a regular basis, with quality-controlled timeseries being released annually for their sites (planning on shifting to quarterly). Eddy covariance flux data from other parts of the world may be compiled and released through an umbrella organization (as in the United States or Australia), but in some cases these efforts are project-based, and not sustained (as in Africa). Some users are still relying on data from the FLUXNET 2015 release, only because there is no other harmonized, global data package.

Regarding the activity data, several respondents indicated that they would like to have more temporal resolution available in the data that they use as input. As an example, fuel consumption data are usually national and annual: more granularity in both space and time would be most welcome. The nightlights product that is used in WP3 used to be available on a monthly basis, but now only annual data are released. Users also reported that the heterogeneity of the activity data in general can be very challenging, due to a range of formats, data sources, gridding, accuracy, and regional coverage.

Some products have historically not been regularly released in NRT, such as TCCON total column measurements. The typical waiting time for these products may have influenced their uptake, with most respondents across the project indicating that these data were used primarily for model evaluation after the fact. As such, this can be seen as something of a chicken-and-egg problem, where data not provided in NRT will not be included in NRT assimilation systems.

This analysis of the timeliness requirements and current availability suggests that the use of NRT *in situ* data within the CO2 Monitoring Service will be very challenging, especially when considering data collected outside of Europe/ICOS. In contrast, many of the remotely-sensed products are already delivering data in NRT. This may result in the NRT operational assimilation relying predominantly on satellite data, with *in situ* data being used more for model evaluation, (re-)analyses, and regional applications. The WMO is working with international partners to coordinate efforts for the timely provision of relevant measurements, but it is unclear on what time scale this effort may bear fruit.

5.2 What’s missing?

Aircraft-based observations of atmospheric composition are not yet included explicitly as an additional category. While they are implicitly included in the discussion of *in situ* measurements of atmospheric mixing ratios of CO_2 and CH_4, they will be explicitly highlighted in the third edition of this report.

High-quality, site-level data on management and site-level ecosystem parameters were highlighted as a missing piece of information that could improve biospheric flux modelling that makes use of these flux data. This is particularly important for heavily-managed land surface types, such as croplands, but is generally relevant. This was to be brought up within the eddy covariance measurement community during a meeting last autumn.

One respondent described a general need for co-sampled meteorology in conjunction with atmospheric composition measurements, and suggested that this needed to be included at more sites. Furthermore, measurement campaigns were identified as being useful to test models, and a need for measurements specifically focussing on vertical profiles and free-tropospheric values was identified. (Here the aircraft-based measurements may play a role.)

Uncertainty estimates, including covariances, on biogenic and anthropogenic emissions were found to be a missing component within the project, but this does not really constitute a measurement as such. Nonetheless, estimates of these uncertainties and covariances, at least for biogenic fluxes, may emerge from the benchmarking efforts of WP5, which are based on observations.

One aspect that is difficult to capture is the need for improved network coverage: while many respondents reported that limited data coverage was one of their main struggles in using the data, there was often little concrete feedback given as to how or where measurement networks could optimally expand. Answering this question more conclusively may require a network design study, which is beyond the scope of these surveys. Some of this information may be derived from modelling studies in WP5 that will feed into Task 7.3, which assesses gaps in the currently available observations.

Referring back to the project overview diagram in Figure 1, it is clear that some observations are also used in WP2 for the production of the flux or emission products that are then used in WPs 3-6. Indeed, perhaps it would be sensible to include another arrow from the “Observations” pillar to the WP2 box. This second iteration of the document included considerably more input from colleagues providing prior flux products in WP2, particularly in terms of anthropogenic emission inventories. This is seen in particular in the discussion of the activity data in Section 4.3.

This deliverable and its successor will serve as a basis for the identification of data providers in Task 7.2, which will then be reported upon in Deliverable 7.5, just as it was done for Deliverable 7.4 in the second year of the project. It will also provide guidance for the development of the prototype of the operational data pipeline in Task 7.4, resulting in Deliverable 7.8.

6 References

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7 List of acronyms

C3S	Copernicus Climate Change Service
CAMS	Copernicus Atmosphere Monitoring Service
CC/FFDAS	Carbon Cycle/Fossil Fuel Data Assimilation System
CDS	Climate Data Store
CGLS	Copernicus Global Land Service
CHE	CO$_2$ Human Emissions project
CHTESSEL	Carbon-Hydrology Tiled ECMWF Scheme for Surface Exchanges over Land
CIF	Community Inversion Framework - A modular system, developed in the VERIFY project, for estimating GHG fluxes.
CLMS	Copernicus Land Monitoring Service
CO2M	Copernicus Carbon Dioxide Monitoring mission
CO2MVS	CO$_2$ Monitoring and Verification Support capacity
CoCO2	Prototype system for a Copernicus CO$_2$ service
CORSO	CO2MVS Research on Supplementary Observations
DLR	Deutsches Zentrum für Luft- und Raumfahrt, German Aerospace Center
ECMWF	European Centre for Medium-Range Weather Forecasts
ECOCLIMAP	A dual database at 1 km resolution that includes an ecosystem classification and a coherent set of land surface parameters
EEA	European Environment Agency
EM27	A solar absorption spectrometer
ERA5	An ECMWF reanalysis data product from 1979 to near real time
ESA	European Space Agency
ESA-CCI	ESA Climate Change Initiative
EVI	Enhanced Vegetation Index
FLUXNET	1) The data portal and 2) measurement site network.
Fr-Tou	Flux tower site in Toulouse
GOME-2	Global Ozone Monitoring Experiment–2
GOSAT	Greenhouse gases Observing SATellite
GPP	Gross Primary Production
GRIB1, GRIB2	GRidded BInary data file formats
IASI	Infrared Atmospheric Sounding Interferometer
ICON	Icosahedral Nonhydrostatic Weather and Climate Model
ICOS	Integrated Carbon Observation System
ICOS ATC	ICOS Atmospheric Thematic Centre
IFS	Integrated Forecasting System - The atmospheric model and data assimilation system at ECMWF
IPCC	Intergovernmental Panel on Climate Change
LAI	Leaf area index
LES	Large Eddy Simulation, a mathematical model for turbulence used in computational fluid dynamics
MARS	Meteorological Archival and Retrieval System

MODIS	Moderate Resolution Imaging Spectroradiometer
MVS	Monitoring & Verification Support
NEE	Net Ecosystem Exchange - NPP minus the heterotrophic respiration
NOAA	U.S. National Ocean and Atmosphere Administration
NPP	Net Primary Production - GPP minus the autotrophic respiration
NRT	Near-Real-Time
NWP	Numerical Weather Production
ObsPack	Observation Package
OCO-2	Orbiting Carbon Observatory 2
OCS	Carbonyl sulfide
PI	Principal Investigator
PROBA-V	PROBA-Vegetation, a satellite in the European Space Agency's PROBA series
SDBM	Simple Diagnostic Biosphere Model
SIF	Solar-Induced Fluorescence
SLIM	Surface Land Information Mapping
SPOT-VEGETATION	Satellite pour l'Observation de la Terre
SYNMAP	A global land cover product
TCCON	Total Carbon Column Observing Network
TERRA	Land surface scheme
TOC	Top Of Canopy
TROPOMI	TROPOspheric Monitoring Instrument
VERIFY	Verifying greenhouse gas emissions project
VOD	Vegetation Optical Depth
VPRM	Vegetation Photosynthesis Respiration Model
WDCGG	World Data Centre for Greenhouse Gases
WMO	World Meteorological Organisation
WP	Work Package
WRF	Weather Research and Forecasting model
XCO_2, XCH_4, and XCO	Total column atmospheric measurements of CO_2, CH_4, and CO

Document History

Version	Author(s)	Date	Changes
0.0	Julia Marshall (DLR)	29/01/2023	First draft complete
1.0	Julia Marshall (DLR)	21/02/2023	Incorporated suggestions from reviewers.

Internal Review History

Internal Reviewers	Date	Comments
Janne-Markus Rintala (ICOS)	06/02/2023	Comments in document, as well as in separate document. Several suggestions to improve clarity of language, and suggestion for restructuring of the next edition for readability.
Richard Engelen (ECMWF)	01/02/2023	Would like to see more concrete quantification of gaps in the current measurement network for the final version.

Estimated Effort Contribution per Partner

Partner	Effort
DLR	1
Total	**1**