Data
Models
Inventories

PARIS

Process Attribution of Regional Emissions

GA 101081430, RIA

Full year of APO data uploaded to the ICOS portal - 1st round

Deliverable D6.2	
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Table of content

1. Changes with respect to the DoA (Description of the Action)

The deliverable has been amended (2nd Amendment of the GA) and covers the APO data uploaded to the ICOS portal through 2024, and associated products derived from the data. The deliverable report provides a brief overview and description of the uploaded data and metadata and is associated to Milestone M43, which describes the methodology and uncertainties associated with the data production and inverse estimates.

2. Dissemination and uptake

The dissemination of D6.2 involves uploading the validated atmospheric oxygen (O_2) and carbon dioxide (CO_2) datasets from two measurement sites in the United Kingdom, for the year 2024, to the ICOS (Integrated Carbon Observation System) Carbon Portal database, where they will be fully accessible to the public. The measurement stations are:

- WAO: Weybourne Atmospheric Observatory, Norfolk (52.95°N, 1.12°E) https://meta.icos-cp.eu/objects/xWsJQmWHFpSYCzOTbhjV9mB2
- HFD: Heathfield Tower, Sussex (50.98°N, 0.23°E) https://meta.icos-cp.eu/objects/olnKJkqvr-PbCshjc0a3yuXm

Making the data publicly available ensures broad dissemination of the O_2 and CO_2 data, allowing stakeholders and the broader scientific community to access and utilize the dataset for various research purposes.

3. Short summary of results

The measurement systems at WAO and HFD are very similar. Continuous, high-frequency (every 2-minutes) measurements of atmospheric CO_2 and O_2 were made at WAO and HFD throughout 2024 using a Siemens Ultramat 6E analyser for CO_2 and an Oxzilla analyser for O_2. The analysers were calibrated approximately every 47 hours following the established protocols of the high-precision atmospheric CO_2 and O_2 measurement communities. Data were quality controlled using a standardised procedure, with code written in R, followed by manual quality assurance, as well as by assessing associated quality control information such as target cylinder results. Data were averaged to hourly values before being uploaded to the ICOS Carbon Portal. For WAO, historical measurements since May 2010 have also been uploaded. For HFD, historical measurements since June 2021 have also been uploaded to the ICOS Carbon Portal. There are no data for 2023 at HFD as the system was not running at that time. At WAO in 2024, there were atmospheric O_2 measurements for 65% of the year, and atmospheric CO_2 measurements for 86% of the year. At HFD in 2024, there were atmospheric O_2 measurements for 70% of the year, and atmospheric CO_2 measurements for 76% of the year. The WAO historical record with a full description of the instrumental setup, methodology and key features of the dataset is published in Adcock et al., 2023.

The PARIS project is developing an inverse modelling framework to derive fossil fuel CO_2 ($ffCO_2$) emissions using simultaneous atmospheric O_2 and CO_2 measurements, combined as the tracer, atmospheric potential oxygen (APO). Preliminary estimates of $ffCO_2$ emissions, based on a comparison of APO-derived estimates of fossil fuel CO_2 mole

fractions and atmospheric simulations were presented in the PARIS Milestone 24 report. A more complete theoretical framework for fossil fuel CO_2 emissions inference using APO was outlined in PARIS Milestone 43. Some *preliminary* results for the PARIS focus country, the Netherlands, is presented here, based on flask sampling from ICOS. The results indicate that the assumed uncertainty associated with the atmospheric transport of APO is likely over-estimated in this version of the inverse model and therefore, combined with the low frequency of the ICOS flask samples, little adjustment of the a priori flux estimate was found. These findings will inform the next version of the inverse model, which will next be applied to the PARIS high-frequency data, and updated results will be presented in a future report.

4. Evidence of accomplishment

The validated atmospheric O_2 and CO_2 data from Weybourne Atmospheric Observatory and Heathfield Tower, in 2024, have been submitted to the ICOS Carbon portal database, where they are fully accessible to the public by specifying the station and species, or by following the links here:

https://meta.icos-cp.eu/objects/xWsJQmWHFpSYCzOTbhjV9mB2

https://meta.icos-cp.eu/objects/olnKJkqvr-PbCshjc0a3yuXm

Evidence shown by the screenshots in the figures 1 and 2 below.

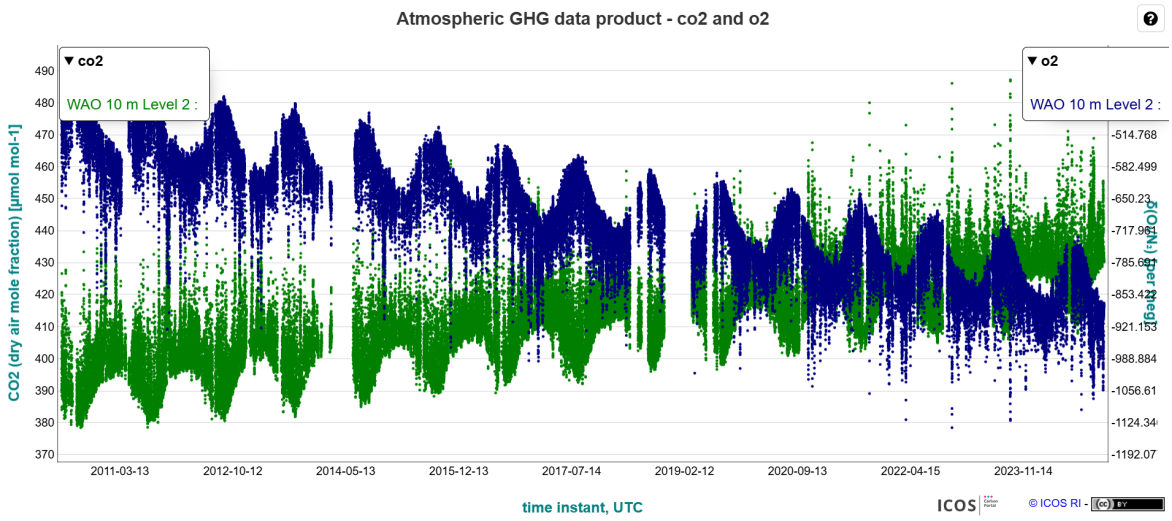

Figure. 1: Screenshot showing uploaded atmospheric O_2 and CO_2 data from Weybourne Atmospheric Observatory (WAO) on ICOS Carbon Portal website.

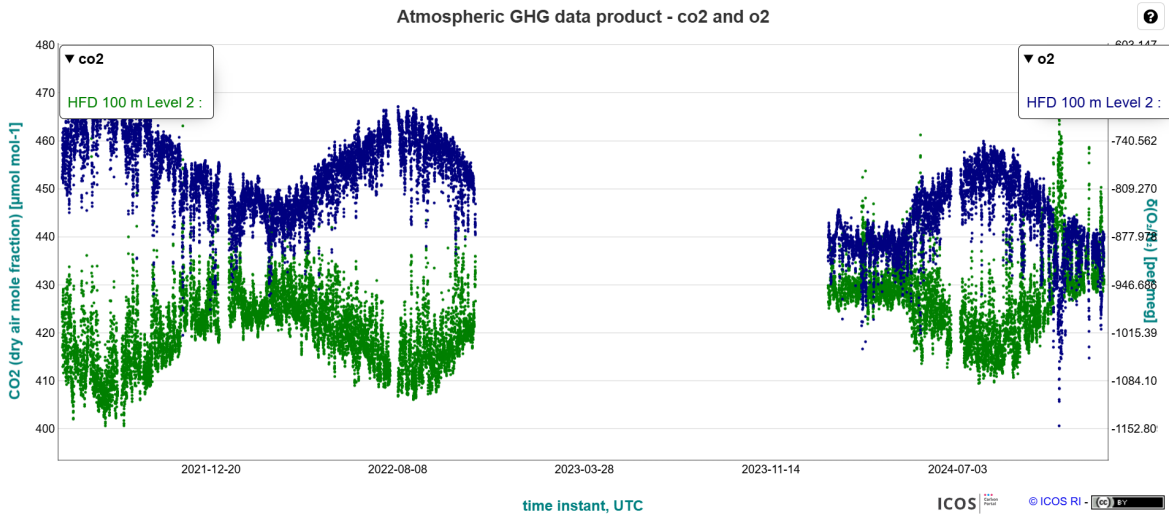

Figure 2: Screenshot showing uploaded atmospheric O_2 and CO_2 data from Heathfield (HFD) on the ICOS Carbon Portal website.

4.1 Introduction

Measurements of atmospheric oxygen (O_2) provide a potentially powerful tool for interpreting changes in carbon dioxide (CO_2), because the oxygen and carbon cycles are tightly coupled. In terrestrial biospheric processes, O_2 and CO_2 are strongly anticorrelated. The atmospheric CO_2 and O_2 measurements can be combined into a tracer known as Atmospheric Potential Oxygen (APO = O_2 + 1.1 × CO_2), which is theoretically invariant to terrestrial biosphere exchange. The coefficient 1.1 represents the mean molar O_2:CO_2 exchange ratio of the terrestrial biosphere. Originally, APO was devised to study ocean carbon-cycle processes, which dominate on seasonal to long-term timescales (Keeling and Manning, 2014). Recent work has shown that it can distinguish between biospheric and ffCO_2 in the atmosphere (Pickers et al., 2022). Details on the measurement methodology and uncertainties were presented in the PARIS Milestone 43 report.

The PARIS project is developing methodologies for inferring fossil fuel CO_2 emissions from observation-derived APO. The theoretical underpinning of this work is described in detail in the PARIS Milestone 43 report. Here, the preliminary results of this version of the system are presented for the Netherlands, which, along with the UK, is one of the two "focus countries" for CO_2 studies in PARIS. For computational reasons, to provide broader spatial coverage, and to provide a comparison to ongoing atmospheric radiocarbon CO_2 inversions from the CORSO project, these preliminary inversions used ICOS flask samples, rather than the high-frequency PARIS data. Results for the UK were omitted because there is no ICOS flask coverage in that part of Europe.

4.2 Scope of the deliverable

Data collection: Measure in-situ atmospheric O_2 and CO_2 continuously with high-frequency (2-min sampling). Ensure the instrument is well-maintained and calibrated regularly.

Data processing and quality control: The bespoke instrument software will collect raw data and also automatically produce calibrated values. Some technical issues will be

automatically recorded in a 'flags' column in the raw data files, while others will be manually recorded in the user log alongside other unautomated metadata. All files produced will be .csv format.

Data documentation: data will be documented on the ICOS Carbon Portal website. Details will include site location and time period, uncertainty of the hourly averages and contact information for the data providers.

Data formatting and standardization: data will be provided as .csv files using ICOS format for missing values, uncertainties, and QC flags. Metadata will be included in the file header.

Data submission to ICOS Carbon Portal database: Submit the standardized observation data files to the ICOS Carbon Portal database following submission procedures and requirements.

Accessibility and data sharing: Ensure that the submitted atmospheric O_2 and CO_2 observation data is fully accessible to the public, including stakeholders and the broader scientific community, through the ICOS Carbon Portal.

4.3 Content of the deliverable

Data description: Time series of continuous atmospheric measurements of O_2 and CO_2: at the Weybourne Atmospheric Observatory between May 2010 and December 2024 (77001 hourly O_2 averages); and at Heathfield Tower between June 2021 and December 2024 (15851 hourly O_2 averages). These measurements are ongoing. The CO_2 is reported in ppm units and was measured using a non-dispersive infrared (NDIR) CO_2 analyser from Siemens Corp., model Ultramat 6E. The O_2 is reported as O_2/N_2 in per meg units and was measured using a dual lead fuel cell O_2 analyser, Oxzilla from Sable Systems International Inc. We report hourly averages of two-minute measurements. An hour must have at least nine measurements or the hourly average is not included. The standard deviations are the hourly standard deviations of the two-minute measurements. Gaps in the data are due to routine running of calibration cylinders, maintenance and removal of data with known technical issues. CO_2 data were transferred onto the WMO NOAA X2019 calibration scale using the linear conversion in Hall et al., (2021). O_2 data are on the Scripps Institution of Oceanography (SIO) 'S2' scale that was used by SIO from April 1995 to August 2017. Full details are provided in Adcock et al., 2023.

Metadata: These datasets are accompanied by comprehensive metadata, detailing information such as the measurement units, station name, and contact information of the data providers.

Findability: These datasets can be accessed via the ICOS Carbon Portal database. Users can locate the dataset by specifying the station (WAO or Weybourne; HFD or Heathfield), and component (O_2 and/or CO_2).

Accessibility: These datasets are publicly accessible through the ICOS Carbon Portal database, ensuring that stakeholders and the broader scientific community can easily access and utilize the data for their research and applications.

Interoperability: The dataset is formatted into standardized .csv files using the ICOS data format, facilitating interoperability with other datasets and platforms.

Reusability: The dataset includes hourly averages with uncertainty, providing a comprehensive view of the observed atmospheric O_2 and CO_2. Atmospheric Potential

Oxygen (APO) can be readily calculated from these data, based on the user's assumptions regarding terrestrial biosphere exchange ratios. The aim is for this data to be reusable for various research purposes and analyses.

Inverse analysis: Figure 3 shows preliminary inversion results for the Netherlands, using APO derived from ICOS flask samples of atmospheric O_2 and CO_2 and the methodology from the PARIS Milestone 43 report. The figure shows that emissions estimates are highly uncertain, with a mean posterior value that is very close to the a priori estimate. The finding that posterior fluxes are very close to the prior likely indicates that transport model uncertainty has been over-estimated in the inversion. Furthermore, the relatively low frequency of the ICOS flask samples may limit the information that can be derived from the data. Future work will focus on reevaluating model uncertainty, continuing to explore reasons for model-data disagreement (e.g., Chawner et al., 2024), and applying the inversion to high-frequency WAO and HFD data in addition to the ICOS flask samples.

Because of the highly preliminary nature of this inversion product, it has not been publicly archived and is shown here to demonstrate the current status of the work.

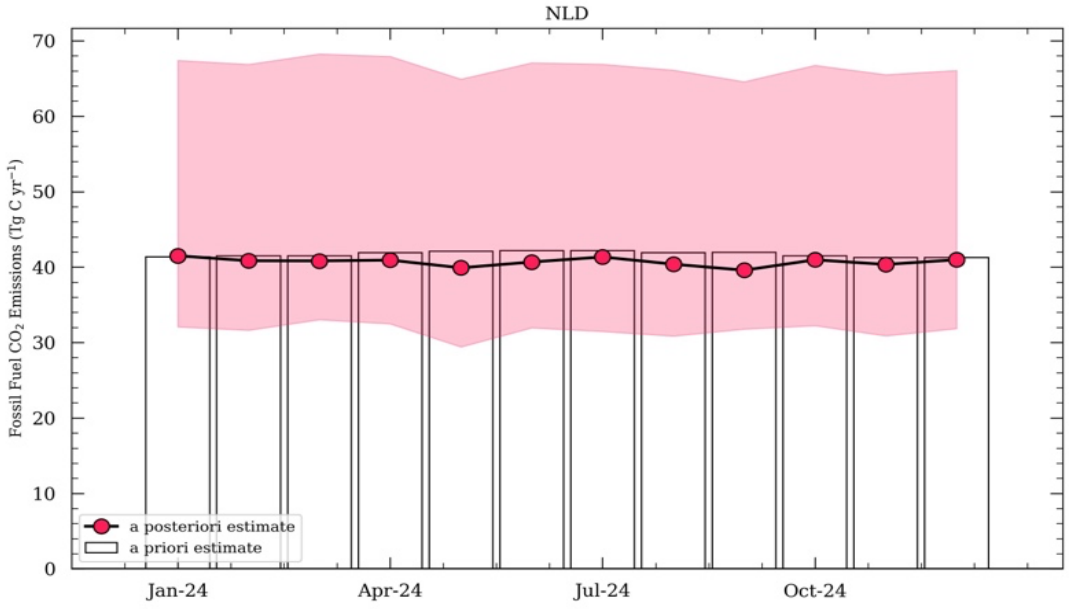

Figure 3: *Preliminary* fossil fuel CO_2 inversion results based on ICOS flask samples of atmospheric O_2 and CO_2 using the methodology outlined in the PARIS Milestone 43 report. The posterior mean emissions are shown as red circles and the shading represents the 68% confidence interval. A priori estimates from EDGAR v8.2 are shown as bars. The small deviation of the posterior results from the prior, combined with the large posterior uncertainty indicates that the inversion is not strongly informed by the data, likely because of the low frequency sampling in the ICOS data and an over-estimate of transport model uncertainty.

4.4 Conclusion and possible impact

The observations of atmospheric O_2 and CO_2 from Weybourne and Heathfield provide detailed and valuable insights into carbon cycle processes including variability of regional fossil fuel CO_2 in the atmosphere in the UK and Europe. These datasets provide valuable information for assessing agreement with similar datasets from other locations and will help contribute to modelling outputs.

The availability of the atmospheric O_2 and CO_2 datasets enhances collaboration and knowledge exchange among consortium members, fostering interdisciplinary research and innovation and serving as a valuable resource for the project. These datasets complement the greenhouse gas (GHGs) emissions data analyzed in other work packages, contributing to efforts on accurately assessing climate change.

By sharing the atmospheric CO_2 and O_2 measurement datasets openly, these datasets facilitate broader scientific inquiry and exploration within the research community, researchers can leverage the data for diverse research applications. These datasets also align with the EU's objectives and priorities related to climate change.

These data have helped to inform the development of the PARIS fossil fuel CO_2 inversion methodology, preliminary results of which have been presented. These preliminary $ffCO_2$ emissions estimates highlight limitations of the existing system, which will continue to be explored, and updates will be presented in future reports.

4.5 References

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5. History of the document

Version	Author(s)	Date	Changes
V 1.0	Karina Adcock	25/11/2025	New document
	Matt Rigby	15/12/2025	Inversion results added
	S. Walter	19/12/2025	Finalizing and upload