CARBON ATMOSPHERIC TRACER RESEARCH TO IMPROVE NUMERICAL SCHEMES AND EVALUATION

Research to Improve Numerics and Evaluation

D5.1 Test bed configuration

Funded by the European Union The CATRINE project (grant agreement No 101135000) is funded by the European Union.

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1 Executive Summary

Within the EU-CATRINE project, we have designed a Testbed that integrates observations, turbulent and cloud simulation results, and global models results obtained at high spatiotemporal resolution. With this Testbed framework, our aim is threefold: (i) to evaluate the global model results with comprehensive observations and turbulent-cloud simulations, (ii) to identify and calculate the main metrics that quantified the transport of greenhouses and (iii) to estimate the causes of systematic errors on the transport of regional and global models, are described and some of them have been finalized. First, and as a proof of the concept of the feasibility of the Testbed, we have selected a three-week measurement campaign in Amazonia [\(https://cloudroots.wur.nl/\)](https://cloudroots.wur.nl/). We have combined observations, highresolution modelling (DALES, 25×25 m² resolution, and the global CAMS model at resolutions, 4.5 , 9 and 27 km²). Second, a list of more than thirty variables have been selected to be intercompared and studied. In combination with the DALES simulations, the observations have enables us to thoroughly evaluate the CAMS model results and identify potential errors on the transport of $CO₂$. Last, from the most representative metrics we will begin to study and quantify the performance of the transport models with respect to the meteorological variables and to carbon dioxide. This will enable us to assess and to quantify errors on the transport, mainly turbulent transport under different thermodynamic conditions, and transport driven by clouds, including the troposphere-stratosphere exchange.

The establishment of the Amazonia Testbed as a proof of concept will be extended to two other ecosystems in which we have already collected comprehensive observations: the transect between Cabauw (grassland) and Loobos (temperate forest) (Ruisdael Campaign May 2022), and the irrigated area surrounded by a semi-arid region in Central Catalonia (LIAISE experimental campaign). Finally, to obtain more robust statistical results on the random and systematic errors, we plan to carry out and extend the intercomparison in the transect Cabauw-Loobos to a complete growing season (from March 2022 till September 2022).

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2 Introduction

2.1 Background

As part of the Copernicus Atmosphere Monitoring Service (CAMS), a new service will be established to monitor emissions of CO2, CH4 and relevant air pollutants, referred to as the CO2 Monitoring and Verification Support (CO2MVS) capacity. The CAMS CO2MVS capacity is targeted for operational status in 2026 in order to provide support to the 2028 Global Stocktake using observations from the CO2M satellite constellation as well as other satellite sensors and in-situ networks. The CATRINE project follows in the footsteps of previous and current H2020 and Horizon Europe projects that were set up to scope, design, develop, and implement prototype systems for the future operational CO2MVS (CHE, VERIFY, CoCO2 and CORSO). CATRINE follows the recommendations from the CHE project to provide improvements and quality control metrics for modelling tracer transport in the CO2MVS which will be crucial for the reliable use of the satellite observations in the operational system.

Uncertainties and errors in the transport of greenhouse gases are often related to the inaccurate representation of unresolved processes, namely the sub-grid processes occurring at smaller spatiotemporal scales than the grid (Schuh and Jacobson, 2023; Yu et al., 2018). These subgrid processes require the use of representations that approximate their physics in form of parametrisations schemes. These processes occur and act at spatiotemporal scales that are smaller compared to the resolved circulation. Representative examples of these parametrisations are the transport driven by dry and moist convective turbulence (mainly clouds)

To quantify these uncertainties and systematic errors we have designed a testbed with the aim of a more systematic manner to find the errors (days-week comparison), and statistically significant process-level evaluation (seasonal comparison). Here, the main purpose is to optimise the identification of large-scale problems that are related to parametrisation schemes of the transport.

The testbed research strategy is divided in two parts (i) a comprehensive comparison of short periods (up to 15 days) with a systematic comparison with numerous observations from field campaigns, operational observing networks and large-eddy simulations, and (ii) intercomparison of representative metrics such as atmospheric boundary layer height or transport driven variables like flux divergence to identify systematic errors.

Two regions of the atmosphere have been selected as the focus of the testbeds: the boundary layer (BL) including the exchange with the free troposphere, and the upper troposphere lower stratosphere (UTLS). These have been identified as areas of priority for the diagnostics of systematic errors as they are subject to large uncertainties and they play a very important role in the vertical transport of tracers (Stephens et al., 2007; Gerbig et al. 2008; Gaubert et al., 2019) across two transport barriers in the atmospheric column, i.e, the boundary layer top (Kretschmer et al., 2012) and the tropopause (Deng et al. 2015), as well as the long-range transport and the inter-hemispheric gradient (Schuh et al., 2019).

Due to the high quality and comprehensive character of the observations two ecosystems have been selected for the BL test beds: the Amazonian rainforest and grasslands and forests in temperate climate conditions. For the upper troposphere, lower stratosphere (UTLS) testbeds around the globe and in different seasons have been chosen. They will be used to assess errors in vertical transport and long-range transport. One common challenge for the transport schemes near the ground and in the UTLS are the high vertical gradients of the trace gases. The strategy for the UTLS is looking into metrics determined from trace gas distributions.

As outlined below, simulations will be performed with DALES, ICON-ART and the IFS models. The IFS model will be the core global model of the CO2MVS, and the ICON-ART model will

be used operationally by DWD and EMPA to monitor the national greenhouse gas emissions. The DALES model has been used previously as part of the Amazon testbed to evaluate Numerical Weather Prediction (NWP) models (Vilà-Guerau de Arellano et al., 2022).

2.2 Scope of this deliverable

2.2.1 Objectives of this deliverables

The aim of this deliverable is to propose a set of Testbeds to (i) evaluate the transport model simulations results with comprehensive observations in the boundary layer and the uppertroposphere and lower stratosphere, (ii) identify and calculate the main metrics that drive transport and (iii) estimate the causes of systematic errors on the transport of regional and global models.

Applied to the rainforest ecosystem the Testbed is currently used to evaluate the large-scale model performance and the identification of the most suitable (objectives 1 and 2). Therefore, it is proven that it is a useful platform to be used to identify random and systemic errors. However, the ultimate aim is to eventually implement those testbeds proposed in this deliverable in an automated manner, so that they can be used operationally to evaluate the atmospheric tracer transport in the CO2MVS.

2.2.2 Work performed in this deliverable.

This deliverable presents the Testbed configuration including all the observations from field campaigns, large-eddy simulations, and global model simulations.

The work performed is explained below with a description of the observations (e.g. Cloud roots in the Amazon), the numerical experiments performed with large-eddy simulations using the DALES model (used previously to evaluate the IFS, Vila-Guerau de Arellano et al. 2020), as well as the global transport simulations to be evaluated from the Copernicus Atmospheric Monitoring Service IFS model and the ICON-ART model used operationally by DWD and EMPA (see the next section for more details). These models are used by ECMWF and the German Weather Office, DWD, to monitor regional greenhouse gases.

Quality controls have been carried out for some of the field campaigns (i.e. in the Amazonia). Regarding the large-eddy simulation 20 numerical experiments were performed to design the case. The testbeds for the UTLS are selected based on available aircraft field campaign data for a range of species (CO2, SF6, q, CH4, CO, O3) and spatial/temporal coverage, considering also the overlap with other global simulations performed as part of the proposed TransCom intercomparison exercise (see Chevallier et al., 2024, D7.1) .

2.2.3 Deviations and counter measures

There are no deviations from the deliverable. The main challenge now is to get the postprocessing of all the data in a correct way to integrate the data.

2.3 Project partners:

3 Description of testbeds

3.1 Observations

3.1.1 Selection of testbeds for atmospheric boundary layer

Figure 1 shows the exact location of the BL testbeds. In selecting the sites, we have been using the following criteria. They are representative sites of key ecosystems, rain and temperate forest, and grassland. The sites are equipped with very comprehensive observations not only on the thermodynamic, but also on greenhouse gases. They include a complete data set of surface observations, but also tower measurements which can be representative of the atmospheric processes. To complete these continuous measurements, at the sites, there have been dedicated campaigns in which soundings and aircraft platforms are used. These observations are key to validate the transport of greenhouse gases. The selected sites are:

1. AMAZON RAINFOREST (Brazil) Stations: ATTO: latitude -2.1458, longitude -59.0055. CAMPINA: latitude -2.1819, longitude -59.0217

2. GRASSLANDS and TEMPERATE FOREST (The Netherlands) Cabauw 213 m tower; latitude 51.963, longitude 4.86 Loobos 50 meter tower: latitude 52.1572, longitude 5.75

3. IRRIGATED and SEMIARiD (Catalonia) LIAISE campaign latitude 41.71, longitude 0.90.

Figure 1. Location of the supersite and intensive field experiments in which the observations used in the testbed were gathered.

A complete description of the observations can be found:

- Amazonia base (Vila-Guerau de Arellano et al., 2024)
- Ruisdael Temperate Forest: Cabauw tower [\(https://ruisdael-observatory.nl/\)](https://ruisdael-observatory.nl/) and Loobos tower [\(https://maq-observations.nl/\)](https://maq-observations.nl/)
- LIAISE (Mangan et al., 2022).

All data sets are very comprehensive and are characterised by observations at tall towers: ATTA-Amazonia (321 m), Cabauw (Temperate-231 m) and Loobostemperate forest (50 m). These standard observations include vertical profiles of state meteorological variables and carbon dioxide. Additional experiments were taken during the *campaign CloudRoots (See Table 1).*

Table 1. Additional measurements to the standard observations taken during the CloudRoots-Amazon 22 campaign (August 2022)

3.1.2 Selection of testbeds for the Upper Troposphere Lower Stratosphere (ULTS)

For all testbeds, the altitude of the tropopause is needed. All simulations with IFS and ICON will be performed in resolutions of 25 km and higher.

Two different periods have been selected:

- 2022- 2023: TransCom period proposed by CATRINE WP7 (see Chevallier et al. 2024, D7.1; see Table 2)
- 2016-2017: ATom and StratoClim field campaigns (see Table 3 and Figure 2)

Testbed	Time	Scope	Gases
OSTRICH - Observations of Stratospheric TRace gases Influencing Climate using High-altitude platforms. https://www.atmo- access.eu/successful-tna- provided-through-atmo- access/	30/07/2023- 11/08/2023	Northern boreal summer	CO2, CO, CH4
MAGIC - Monitoring Atmospheric composition and Greenhouse gases through multi-Instrument Campaigns https://www.data- terra.org/en/news/magic- greenhouse-gases/	Autumn 2022 and 2023	Northern mid latitudes	CO2, CO, CH4, H2O
AIRCORE Bolivia https://www.gml.noaa.gov/cc gg/aircore/	August 2023	Southern low latitudes	CO2, CO, CH4, H2O
PHILEAS - Probing High Latitude Export of air from the Asian Summer Monsoon https://halo- research.de/sience/previous- missions/phileas/	August and September 2023	Northern high and mid latitudes	To check what is available when all retrievals are finished
DCOTSS - Dynamics and Chemistry of the Summer Stratosphere https://asdc.larc.nasa.gov/pr oject/DCOTSS	End of May to beginning of June 2022	Continental USA; overshooting convection	CO2, CO, CH4, H2O

Table 2: List of UTLS testbeds covering period from 2022 to 2023

All testbeds from above will be supported by measurements from the ACE satellite and from IAGOS-CORE observations. For the DCOTSS campaign there are nearby IAGOS-CORE flights after the overshooting event which will be used to investigate the transport after the overshooting event. For the PHILEAS campaign, biomass burning products (e.g., PAN) will also be used and compared to artificial tracers in the model to determine long range transport from the wildfires that happened during this summer.

Testbed	time	Scope	Gases
StratoClim https://halo- db.pa.op.dlr.de/missi on/101	Aug/Sep 2016 and July/Aug 2017	Mediterranean and Himalayan	CO, CO2, H2O, SF6
Atmospheric Tomography Mission (ATom) https://daac.ornl.gov/ <u>cai-</u> bin/dataset_lister.pl? $p = 39$	Aug 2016 to Oct 2017	global, all seasons (see figure 2)	CO, CO2, CH4, H ₂ O, O ₃ , SF ₆

Table 3: List of UTLS testbeds covering period from 2016 to 2017

Here, only one simulation will be done to cover everything. Additionally, further observations during this time frame will be used where useful (e.g., from CONTRAIL and CARIBIC aircrafts).

Figure 2: (top left) Map of the flight tracks and stops for the four ATom deployments (top right) Density matrix aggregating the entire 1-Hz dataset for ATom-1–4 illustrating the data coverage achieved for the campaign (bottom) Flight track of ATom-3 shown as an example of the tomographic vertical profiling pattern; from Thompson et al. (2021)

For the UTLS, different observations from different instruments (e.g. AirCore, GLORIA, FISH, COLD2, HUPCRS, IAGOS-CORE Package1 and Package2d) will be used. They are comprehensive and taken at different temporal scales (seconds to minutes). For better comparison, those observations will be averaged to the same temporal resolution. As the tropopause acts as a transport barrier (resulting in high gradients of gases) and we cannot expect the tropopause in the models to be at the same height as in the real world, profiles relative to tropopause altitude will be created.

3.2 Large-eddy simulation DALES

Table 2 provides a list of the numerical experiments performed using the large-eddy simulations

Testbed	Dates	Domain	Resolution
Amazon rainforest	09, 10, 11, 14, 15, 50 x 50 km2 17 18 August 2022 (7 days)		50 x 50 x 20 m
Ruisdael Temperate Forest/Cabauw tower	17-18 May 2022 Growing season	150 x 150 km2	100 x 100 x 20 m3
Irrigated/semi-arid test bed	15 - 31 July 2021	100 x 100 km2	60 x 60 x 20 m3

Table 2: List of LES Numerical Experiments carried out with DALES for each testbed

To design the numerical experiment, we have done 30 numerical experiments to determine and to adjust the initial and boundary conditions. In all the experiments the observations have constrained the values.

3.3 Simulations using IFS and ICON-ART

The aim of the testbeds is to provide a process-based evaluation of CO2MVS transport model developments in the boundary layer and UTLS. The Integrated Forecasting System at ECMWF is the core global model of the future CAMS CO2MVS, and therefore a lot of emphasis is put on the evaluation of the IFS using the operational configuration of the model for CAMS (currently CY49R1). Sensitivity experiments with new parametrization developments, such as the TKE scheme, and the Stochastically Perturbed Parametrizations scheme will be used to assess the different sources of uncertainty. Finally, intercomparisons with the ICON-ART simulations will also provide very valuable information as an independent reference. Table 1 lists the planned experiments that will be evaluated using the testbeds described above.

Table 1: List of experiments to be compared with observations and large-eddy simulation numerical experiments.

IBelow, we present the IFS resolutions and frequency of model output (also ICON):

- Tco399 (25km) 3-hourly output
- Tco1279 (9km) 3-hourly output
- \bullet Tco2559 (4.5km) 1-hourly output
- The model runs with ICON-ART will be done with a resolution as close as possible to the IFS resolutions. For the higher resolutions, the runs will be done in a nested mode using the coarser resolution simulation as boundary condition.

CAMS emissions are prepared for IFS and ICON. They are used in the same way in both models. In the chosen ICON simulations, ICON results will be compared using its own dynamics to model runs where meteorology from ECMWF is used as boundary condition. This should help distinguishing between errors introduced due to meteorology and errors due to the transport scheme.

4 Results

4.1 Evaluation observations, LES and CAMS

We have started to analyse and intercompare the data. A representative example is presented in Figure 3. There we show the observations, large-eddy simulations, and IFS model. Statistics of the performance are reported. These results are extended to all the variables under study (listed in Appendix). An important part of the strategy is to interrelate variables to establish cause-effect relationships. Here the strategy is to analyse the intermediate variables used in the parameterizations of key variables that drive and characterize the transport of greenhouse gases. Representative examples are the boundary layer height, the exchange flux between the atmospheric boundary-layer and the free troposphere, and the transport (mass flux) by clouds. In doing so, we can determine the accuracy and reliability of the IFS and ICON parameterizations in reproducing processes relate to the variables, and to quantify the errors associated to miscalculations.

Figure 3. Left: sensible heat flux above the rainforest. Right: evolution of the potential temperature. The observations are an aggregate of six days characterised by the presence of shallow cumulus. The shading is the variability of the six days.

4.2 Metrics to determine errors in the transport.

Our main aim is to select metrics that enable us to identify systematic errors in the transport from the list of the variables presented in the Appendix. Here, we focus on the intertwined relation between variables. We use an example that is presented in figures 4 (intermediate variables) and 5 (mass flux and cloud cover) (Vila-Guerau de Arellano et al., 2024). In designing the Testbed, our aim is to use a similar strategy with the IFS and ICON-ART models results. In this figure we present the main surface and turbulent variables that control the mass flux due to the presence of clouds between the atmospheric boundary layer and the free troposphere. This process is key in the ventilation of greenhouse gases. Key in the figure is the combination of comprehensive observations and a surrogate of a regional model. The aim is to complete this figure using the IFS and ICON high resolution model results.

Figure 4. Sequence of all the variables used to calculate the area fraction of the cloud core and the mass flux at cloud base. Results are presented for the aggregates of the shallow cumulus (ShCU) and shallow-to-deep convection (ShDeep). The variables are calculated using the observations (xaxis) or the rainforest-atmosphere coupled model (y-axis). The variables are: (a) time of a parcel to move upwards from the canopy top to the atmospheric boundary layer height calculated from the atmospheric boundary layer height and the convective velocity (z_i/w·), (b) entrainment velocity (dzi /dt), (c) transition layer defined as lifting condensation level minus the atmospheric boundary layer height (Δz), (d) infinitesimal discontinuity (jump) at the ABL (Δq^2), (d) difference between total and saturation specific humidity (q_t_q_s), and (f) variance of the specific humidity (σ^2 q). Δq is the difference between the specific humidity in the free troposphere and the ABL.

Figure 5 (a) Area fraction of cloud core a_{cc} and (b) mass flux expressed as a velocity M. The calculations are based on observations (x-axis) and the coupled rainforest-atmosphere model (y-axis). They correspond to six-day aggregates of shallow cumulus (ShCu) and four-day aggregates of deep convection (ShDeep). Figure 4 shows the intermediate variables that are used for the calculations of a {cc} and M. A similar strategy will be used in the TestBed to compare the IFS and ICON ART variables.

Other metrics that will be used will be the atmospheric boundary layer height and the advective and turbulent diffusive flux.

4.3 Causality in systematic errors

This section is included as the last part of the design of the Testbed. It only shows our plan and methodology to be used once all the observations, LES and large-scale models are evaluated, and the main metrics are calculated (see sections 4.1 and 4.2).

Once we identify the key metric that quantify the transport of CO2 (in the equation represented by C), we need to quantify the errors and the dependence on other atmospheric physical and composition variables (in equations below represented by ϕ).

Here we propose to take an approach like the one proposed by Pino et al. (2012). In short, we can quantify the errors using:

$$
\text{RSC}_{\phi} = \frac{\partial C}{\partial \phi} \cdot \frac{\phi}{C},
$$

$$
RSF_{\phi} = \frac{\partial \langle \overline{w'c'}|_{s} \rangle}{\partial \phi} \cdot \frac{\phi}{\langle \overline{w'c'}|_{s} \rangle}
$$

using normalised (Relative) Sensitivity to the mixing ratio molar fraction C (RSC), and the relative Sensitivity of Flux (RSF).

Figure 6 presents an example of the sensitivity of the surface flux of carbon dioxide to variables that determine the boundary layer height. The figure clearly marks the influence of the diurnal variability on the carbon dioxide surface flux with respect free tropospheric conditions

represented by ($\gamma\theta$) and the initial (morning) conditions at the inversion ($\Delta\theta$ o). After 10:00 UTC, the rapid growth of the boundary layer yields to a faster increase with time of the absolute value of this sensitivity; that is, the conditions at the free atmosphere represented by the sensitivity to the values of the potential temperature lapse rate $(y\theta)$ are important to infer the $CO₂$ surface flux.

Figure 6. Time evolution of the sensitivity of inferred surface flux of CO₂ to initial value of the CO₂ mixing ratio in the free atmosphere (figure 8 from Pino et al, (2011). The figure shows the sensitivity of the surface flux w'c's as a function of the initial concentration of $CO₂$ in the free troposphere.

We plan to extend this sort of analysis using the model results from IFS and ICON.

5 Conclusion

The Testbed configuration is ready to be used to identify the accuracy and precision of the transport of greenhouse gases in carbon-regional/global models. In designing the Testbed we have focused on integrating and visualising three main components: (1) comprehensive observations, (2) large-eddy simulations that explicitly calculated the transport by turbulence and clouds, and (3) the high-resolution of the CAMS model.

The first Testbed results based on the transport of carbon dioxide during the dry season in the Amazon rainforest is currently under analysis. The analysis includes first comparing and validating radiation and surface processes, diurnal variability of wind, potential temperature, specific humidity and carbon dioxide and their vertical profiles. In this report, we have also included the plan to study in more detail the performance and errors in the representation of the CO2-tramsport. Here, our plan is to study the performance of key metrics that characterize the transport and mixing of carbon dioxide: atmospheric boundary layer, flux divergence, and the mass flux of clouds. The final stage is the estimation of the source of errors in the transport $CO₂$.

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Annex 1

List of variables to be compared for the IFS, ICOPN, LES and the available observations

Surface properties

- 1. Soil Moisture (swvl) at all levels available
- 2. Soil Temperature (skl) at all levels available
- 3. Skin temperature (skt)
- 4. Leaf Area Index (lai_hv and lav_lv) for high and low veg
- 5. Vegetative cover (cvh, cvl) for low and high veg
- 6. Type of vegetation (tvl and tvh) for low and high veg
- 7. Soil type (slt)
- 8. Albedo (al)
- 9. Surface roughness (momentum fsr and heat flsr)
- 10. 2 m temperature and humidity (t2m, d2m (or whatever humidity variable is available)
- 11. 10 m wind (u10, v10)
- 12. Surface Pressure

Radiative and Energy Fluxes (including CO2. CH4, CO) at surface

- 1. SWin (ssrd), SWout, LWin, LWout (or Rn) (ssr)
- 2. G (this might be a residual if it is not printed explicitly) (gflux, 26018, can be computed as residual)
- 3. H (sshf)
- 4. LE (slhf) (do you have the partitioning between soil and plant
- 5. Friction velocity (zust 228003)
- 6. NEE (Farquhar and if possible Ags for CloudRoots (all days) and Cabauw (17-18 May)
- 7. GPP (Farquhar and if possible Ags)
- 8. Soil respiration

Meteorological and carbon variables (in isobararic and z coordinates from surface stratosphere) :

- 1. Divergence (d)
- 2. specific humidity (qt)
- 3. water variables: qv, ql, qi, qr, qs (only qv,ql,qr are necessary)
- 4. air temperature (t)
- 5. dew point
- 6. 3 wind (u, v, and w components)
- 7. K diffusion coefficient (heat)
- 8. Turbulent Kinetic Energy (not available without TKE scheme)
- 9. Radiative heating
- 10. Air density (can be computed with postprocessing)
- 11. Vorticity
- 12. WVPD (can be computed with post processing)
- 13. CO2
- 14. CH4

15. CO

Atmospheric Boundary Layer and Cloud Variables

- 1. Exchange coefficient K (turbulent diffusion coefficient for heat)
- 2. Atmospheric boundary layer height (blh)
- 3. Cloud base height
- 4. Height of convective clouds
- 5. Cloud base cbh
- 6. Cloud top hcct
- 7. Cloud cover
- 8. Cloud type (stratiform/convective)
- 9. Liquid water content (column)
- 10. Rain
- 11. CAPE and CIN

UTLS Variables

- 1. Carbon dioxide (CO2)
- 2. Carbon monoxide (CO)
- 3. Methane (CH4)
- 4. Ozone (O3)
- 5. Water vapor (H2O)
- 6. Sulfur hexafluoride (SF6)
- 7. Temperature
- 8. Air pressure
- 9. Cloud cover
- 10. 3d wind

Document History

Internal Review History

