CARBON ATMOSPHERIC TRACER RESEARCHTO IMPROVE NUMERICAL SCHEMES AND EVALUATION

D7.1 Design of protocol for preliminary global model intercomparisons

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1 Executive Summary

This deliverable defines the framework for a high-resolution atmospheric transport model intercomparison exercise. The aim is to use model configurations with the equivalent of 100-km grid cells or finer horizontally and at least 50 layers vertically. The simulations of four tracers, CO_2, fossil CO_2, SF_6 and ^{222}Rn, will be evaluated using reference observations including ground-based or satellite retrievals and air-sample measurements from tall towers, aircraft and AirCore soundings. Simulated correlations between tracers will be compared with each other, as will vertically integrated mass fluxes for total column. Metrics will be defined to score model performance, considering factors like vertical resolution. Diagnostics will focus on transport errors' impact on the seasonal cycle at different layers and total column, aiding error attribution. The high-resolution simulation database will have broad applications beyond model evaluation, potentially including model uncertainty quantification and AI training. This initiative, originating from the European project CATRINE, seeks global participation from other partners to contribute expertise and models.

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2 Introduction

2.1 Background

Monitoring the greenhouse gases carbon dioxide (CO_2) and methane (CH_4) from space has made great strides over the past decade, in particular in terms of imaging capability. Existing instruments for CO_2 include NASA's Orbiting Carbon Observatory-2 (OCO-2) with continuous sampling of cloud-free regions along the orbital path at a resolution of 3 km^2, and NASA's OCO-3 which introduced the possibility of performing successive side-by-side scans of small areas (~80 × 80 km^2). For CH_4, the TROPOMI instrument on board Copernicus Sentinel-5P provides near-daily surface coverage of cloud-free regions at a spatial resolution of up to 38.5 km^2. In addition, retrieval capabilities at higher spatial resolution are emerging, for instance from Copernicus Sentinel-2 or from Greenhouse Gases Satellite (GHGSat). In the near future, the Copernicus CO_2 Monitoring Mission (CO2M) will extend the imaging capability of CO_2 to a level comparable to the existing one for CH_4 from TROPOMI. This new wealth of CO_2 and CH_4 satellite retrievals pushes the application of such satellite data towards the inference of anthropogenic emissions and absorptions, with target spatial scales much finer than the traditional zonal or subcontinental scales of global atmospheric inversions. In this regard, the current generation of global atmospheric transport models that operate primarily at resolutions coarser than one degree, risks obsolescence because most models cannot exploit the higher resolution information in which most of the anthropogenic signals reside.

2.2 Scope of this deliverable

2.2.1 Objectives of this deliverables

Here, we aim at stimulating high-resolution tracer transport modelling by setting-up a dedicated intercomparison exercise. By “high-resolution”, we first mean the equivalent of a grid spacing of 100 km in the horizontal, or a minimum of 51,000 horizontal grid points (about 1 degree × 1 degree resolution in the Tropics) to pave the world. On the vertical, we put a simple lower limit of 50 layers between the surface and the top of the atmosphere, assuming that it implies sufficient refinement of the planetary boundary layer and around the tropopause for constructive intercomparison. Indeed, the model vertical profiles will be particularly looked at in this exercise. We expect that their evaluation for several tracers using observed profiles from tall towers, aircraft and AirCore soundings will shed some light into the current discrepancies of atmospheric inversions that assimilate column retrievals or air-sample measurements.

Tracer transport simulations will be prepared at such “high resolution” under a common protocol, compared together and with independent observations and made available publicly. We will study CO_2, sulfur hexafluoride (SF_6) and the radon isotope ^{222}Rn. In addition, we will consider the transport of the imposed fossil CO_2 emission fields.

Simulated tracers will be compared with each other, as will vertically integrated mass fluxes for total column. The reference observations will be diverse: ground-based or satellite tracer retrievals, air-sample measurements, as well as meteorological observations. We will define metrics to score the model performance. We will investigate how model configuration, like the vertical resolution, influences the model skill. The diagnostics will be applied to all tracers on weekly to monthly timescales, focusing on the impact of transport errors on the seasonal cycle at various layers and the total column. The correlation between the errors in the different layers with the error in the total column will support the attribution of the transport error.

The high-resolution simulation database will be the first of this sort and may serve various applications beyond the planned model evaluation, from, e.g., model uncertainty quantification to AI training.

This initiative originates from the European project Carbon Atmospheric Tracer Research to Improve Numerics and Evaluation (CATRINE), which funds the coordination of the intercomparison, as well as some contributors, but it is hoped that other partners in the world will join the momentum and contribute to the study with their respective model and expertise.

2.2.2 Work performed in this deliverable

The emphasis on high-resolution global simulations implies strong technical constraints in terms of computing resources and disk space. The protocol is therefore a compromise between (i) the expected richness of the generated content, (ii) the volume of data to be generated (excluding the data from the spin-up period), then transferred and archived, and (iii) the effort to generate them. In particular, we tried to keep the volume of data for most expected submissions within a few terabytes.

2.2.3 Deviations and counter measures

None.

2.3 Project partners:

Partners	
EUROPEAN CENTRE FOR MEDIUM-RANGE WEATHER FORECASTS	ECMWF
COMMISSARIAT A L ENERGIE ATOMIQUE ET AUX ENERGIES ALTERNATIVES	CEA
METEO-FRANCE	METEO-FRANCE
WAGENINGEN UNIVERSITY	WU
KARLSRUHER INSTITUT FUER TECHNOLOGIE	KIT
HELSINGIN YLIOPISTO	UH
UNIVERSITE DE REIMS CHAMPAGNE-ARDENNE	URCA
ALBERT-LUDWIGS-UNIVERSITAET FREIBURG	UFR

3 Modelling protocol

3.1 Imposed configuration

3.1.1 Spatial resolution

The models used for the submissions have to pave the whole globe with at least 51,000 horizontal effective grid points, or an equivalent resolution in the case of spectral models. 51,000 is the number of 100^2 km^2 cells that are needed to pave the 510 million km^2 of the Earth surface. In the vertical, the lower limit is set at 50 levels, but coarser resolutions are accepted if they represent a sensitivity experiment around a reference version with more than 50 levels in the vertical.

Submissions with the same model at several high resolutions are encouraged.

3.1.2 Period covered

The target period goes from 1 January 2022 at 00:00 UTC until 31 December 2023 at 24:00 UTC. This period will be preceded by one month spin up, starting from initial conditions provided (see section 3.1.5).

3.1.3 Simulated tracers

The intercomparison will study CO_2 as the key tracer, SF_6 for large-scale transport properties and ^{222}Rn for short-range transport properties. In addition, it will consider the transport of the imposed fossil CO_2 emission fields (described in the next subsection) separately in the form of a separate tracer.

3.1.4 Surface fluxes

All surface fluxes will be made available publicly on https://thredds-su.ipsl.fr/thredds/catalog/tgcc_thredds/work/p24cheva/CATRINE/catalog.html.The surface fluxes of CO_2, SF_6 and ^{222}Rn are imposed as follows:

For CO_2

In the base version, they are defined from a disaggregation of CAMS fluxes optimized with OCO-2 land retrievals, on a 0.1° grid.

A second, optional, version will use a disaggregation of the mean of the future Global Carbon Project’s Global Carbon Budget 2024 inversions, on a 0.1° grid.

For fossil CO_2

They are defined monthly from the maps of variable TOTAL of group CO_2 in GridFEDv2024.1 (when available, current on https://zenodo.org/records/8386803). The interpolation of the native 0.1° grid to the model grid, made by each model contributor, has to conserve mass.

For SF_6 emissions

They are defined annually from the maps of variable with long_name TOTALS of EDGARv8.0, available from https://edgar.jrc.ec.europa.eu/dataset_ghg80, with data for 2022 used for 2023 as well. The interpolation of the native 0.1° grid to the model grid, made by each model contributor, has to conserve mass. In addition, Each contributor has to scale the 2022 and 2023 global annual totals in order to match the growth rates reported by NOAA (https://gml.noaa.gov/webdata/ccgg/trends/sf6/sf6_gr_gl.txt).

For ^{222}Rn

In the base version, they are defined monthly from Zhang et al, (2021) available from http://ftp.as.harvard.edu/gcgrid/data/ExtData/HEMCO/ZHANG_Rn222/v2021-11/. A second, optional, zonal annual mean emissions used in a previous TransCom intercomparison (Patra et al., 2011). The interpolation of the native 0.5° grid to the model grid, made by each model contributor, has to conserve mass.

3.1.5 Initial tracer state

Realistic initial states for CO_2 and SF_6 are imposed on 1 December 2021 at 00:00, allowing one month of spin-up before the target period. Both states are defined from LSCE inversions (CAMS product in the case of CO_2). They will be made available publicly on https://thredds-su.ipsl.fr/thredds/catalog/tgcc_thredds/work/p24cheva/CATRINE/catalog.html.

For fossil CO_2, contributors are asked to start from a null state (or from a given constant value) on 1 January 2022 at 00:00.

For ^{222}Rn, contributors are asked to start from a null state (or from a given constant value) on 1 December 2021 at 00:00.

3.1.6 Data policy

The submitted data of the transport simulations will be evaluated internally together with the data providers. Quality-controlled data will be distributed freely and publicly via the CATRINE web site (likely live at the end of May). Users of the data will be encouraged to give fair credit to the contributors and contact them.

3.2 Compulsory outputs

3.2.1 File format

The submitted data files need to be in NetCDF4 format, with the float variables stored in single precision (32 bits).

3.2.2 3D variables

The following 3D instantaneous variables need to be provided every 3 hours for the full target period at a spatial resolution consistent with the model configuration.

- CO_2, fossil CO_2, SF_6 and ^{222}Rn dry air mole fractions

A clear definition of the corresponding vertical pressure grid and horizontal grid needs to be provided, together with the area of the horizontal grid cells at the surface.

3.2.3 2D variables

The following 2D variables need to be provided every 3 hours for the full target period at a spatial resolution consistent with the model configuration.

- The instantaneous surface pressure (Pa),
- The instantaneous planetary boundary layer height (m),
- The instantaneous tropopause height (m).
- Time integrated (over 3 hours), vertically integrated northward (F_N) and eastward (F_E) tracer flux (kg/m) for the total column:

$$F_N = \frac{1}{g}\int_0^{p_s} v\, q_c\, dp \qquad \text{and} \qquad F_E = \frac{1}{g}\int_0^{p_s} u\, q_c\, dp$$

where q_c is the tracer mixing ratio (kg/kg), u and v are the zonal and meridional wind components (m/s), p (Pa) is atmospheric pressure, p_s is the surface pressure, g (m/s^{-2}) is the gravitational acceleration.

- Time integrated (over 3 hours), vertically integrated tracer divergence flux D (kg m^{-2}):

$$D = \nabla.(F_N + F_E)$$

The vertically integrated mass fluxes and their divergence are accumulated over time period of 3 hours so that they can be used to estimate vertical column budgets:

$$\frac{dm_c}{dt} = -D + E - S$$

where m_c is the total global mass of the tracer, D is the time-integrated vertically integrated tracer divergence flux and E and S are the time-integrated vertically integrated emissions and sinks respectively.

The submission needs to explain how the planetary boundary layer height and the tropopause height have been computed.

3.3 Optional outputs

The 3D specific humidity (kg/kg) and associated 2D fluxes described in Section 3.2.3 above will be used as well in the intercomparison when available, with the same time-space resolution specifications as above.

4 Preliminary participant list

Model	Institute/ consortium	Online/ Offline	horizontal	vertical	Driving meteorology	Contact person
ICON-ART	KIT	Online	80/ 13 km	90, 120 levels	ERA5	Stefan Versick
IFS	ECMWF	Online	25/ 9 km	137 levels	ERA5	A Agustí-Panareda
LMDZ	CEA	Both	90 km 44 km 22 km	79 levels	ERA5 (nudging)	F Chevallier and Adrien Martinez
TM5	WU	Offline	1° times 1°	25, 34 up to 137 levels	ERA5	Wouter Peters and Maarten Krol

5 References

Zhang, B., Liu, H., Crawford, J. H., Chen, G., Fairlie, T. D., Chambers, S., Kang, C.-H., Williams, A. G., Zhang, K., Considine, D. B., Sulprizio, M. P., and Yantosca, R. M.: Simulation of radon-222 with the GEOS-Chem global model: emissions, seasonality, and convective transport, Atmos. Chem. Phys., 21, 1861–1887, https://doi.org/10.5194/acp-21-1861-2021, 2021.

Patra, P. K., Houweling, S., Krol, M., Bousquet, P., Belikov, D., Bergmann, D., Bian, H., Cameron-Smith, P., Chipperfield, M. P., Corbin, K., Fortems-Cheiney, A., Fraser, A., Gloor, E., Hess, P., Ito, A., Kawa, S. R., Law, R. M., Loh, Z., Maksyutov, S., Meng, L., Palmer, P. I., Prinn, R. G., Rigby, M., Saito, R., and Wilson, C.: TransCom model simulations of CH_4 and related species: linking transport, surface flux and chemical loss with CH_4 variability in the troposphere and lower stratosphere, Atmos. Chem. Phys., 11, 12813–12837, https://doi.org/10.5194/acp-11-12813-2011, 2011.

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