



CO₂
Human
Emissions

Regional nature runs

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che-project.eu



Co-ordinated by
 ECMWF



CO₂ Human Emissions

D2.4 Part I: Regional nature runs

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1 Executive Summary

This report presents the high-resolution nature runs covering a domain centred around the town of Berlin. These nature runs are nested in the European runs (described in the first part of Deliverable D2.4), themselves nested in the global Tier-1 runs (Deliverable D2.2). These simulations are produced using two separate models, COSMO-GHG and LOTOS-EUROS. COSMO-GHG computes the meteorology and tagged tracers for multiple anthropogenic and biogenic sources. The meteorological outputs drive the offline model LOTOS-EUROS, which computes reactive trace gases and aerosols on top of the tagged tracers.

2 Introduction

The CO₂ Human Emission (CHE) project has been tasked with providing a library of simulations that can be used as a reference -- referred to as nature run -- in Observing System Simulation Experiments (OSSEs) for the exploration and design of future space-based carbon observing systems. The library of runs covers multiple scales and models, from the global scale (described in the Deliverable D2.2), down to the European scale (described in the first part of the deliverable D2.4) and to the local scale, presented here.

These high-resolution (1 km) runs cover a limited area including Berlin as well as several high emitting power plants. The focus is on the description of the simulation setup as well as an illustration of the benefit of the high-resolution in the capability of simulating, localising and following plumes from large point sources.

2.1 Background

One of the critical elements of a European contribution to a global "CO₂ emission monitoring system" identified in the CO₂ report commissioned by the European Commission (Ciais et al., 2015) is a constellation of CO₂ satellites with imaging capability. Between 2011 and 2015, ESA conducted a detailed Phase A/B1 assessment for the CO₂ imaging satellite concept CarbonSat (Bovensmann et al., 2010). In several science studies (LOGOFLUX-1, 2014; LOGOFLUX-2, 2015, SMARTCARB, 2017-2018) supporting this assessment, it was demonstrated that such a satellite would allow observation of CO₂ plumes of strong localized sources such as large cities and power plants and would help constrain emissions at the regional and national scale (Broquet et al. 2018, Brunner et al. 2019, Kuhlmann et al. 2019). However, such emission quantification faces substantial challenges due to the limited precision of the satellite measurements, systematic biases introduced by incompletely accounting for the effects of aerosols and other factors in the retrieval, the limited spatial and temporal coverage and resolution of the observations, and the difficulty in separating the signals from natural CO₂ fluxes from those of anthropogenic emissions.

To support the assessment of the requirements for a future space mission and the challenges introduced by the issues listed above, a library of realistic CO₂ simulations for present-day and future emission scenarios, from the global to the regional and point-source scale is needed.

WP2 of the CHE project aims at producing such a library of simulations mimicking reality as closely as possible, so-called nature runs. This task involves six different institutes running five different atmospheric transport models. The first version of the global simulations has already been completed and is described in the Deliverable D2.2. The updated version of these simulations will be available soon. The European nature runs have also been completed and are used as boundary conditions for the regional runs around Berlin.

2.2 Scope of this deliverable

2.2.1 Objectives of this deliverables

The objectives of this deliverable are to present the setup of the high-resolution regional nature runs, report on the progress of the simulations and show some comparisons with simulations at lower resolution.

2.2.2 Work performed in this deliverable

A year-long high-resolution simulation of meteorology and tagged tracers has been performed with the model COSMO-GHG for 2015, as well as two months (February and July) of offline chemistry and aerosol simulation with the model LOTOS-EUROS.

2.2.3 Deviations and counter measures

The original deliverable D2.4 was supposed to cover both European and regional runs and be delivered at month 21. Due to delays, it has been decided that the European runs would be described in a separate part of deliverable and that the present one would only cover the Berlin simulations. The other set of regional simulations, covering Beijing and Shanghai, will be described in the deliverable D2.7 studying the impact of aerosols, since only this single task depends on these simulations.

3 Model configuration

The precise model configuration has been described in the deliverable D2.1. However, some minor changes have occurred since. We therefore briefly recollect the key components of these simulations.

3.1 Models

3.1.1 COSMO-GHG

The Consortium for Small-Scale Modelling (COSMO) is a consortium of seven European national weather services formed in October 1998 which aims to develop, improve and maintain a non-hydrostatic limited area atmospheric model. The COSMO model is used for both operational and research applications by the members of the consortium, universities and research institutes.

The COSMO-GHG model is an extension of COSMO with modules for the passive transport of greenhouse gases (GHG). The extension builds on the tracer module, which was developed for COSMO to provide a flexible mechanism for incorporating passively transported tracers (Roches and Fuhrer, 2012). The tracer module has been fully integrated in the latest official COSMO version 5.6a, which is parallelised on GPU. COSMO-GHG includes additional routines for simulating a set of tracers which are not only passively transported but also experience the influence of three-dimensional emissions or surface fluxes read in from external datasets (Liu et al., 2017) or computed online (Jaehn et al., 2020).

For the simulations covering the domain around Berlin, COSMO-GHG uses a rotated pole projection to define its simulation grid, whose pole is the same as for the European simulation. The size of the model domain is specified as 670 × 600 grid cells with a resolution of 0.01° (~1.1 km) and 60 vertical levels. The size of the domain is thus 740 km × 670 km.

- Rotated pole: lon = -170° ; lat = 43°
- startlon = -1.4°
- startlat = 2.5°

- $dlon = 0.01^\circ$
- $dlat = 0.01^\circ$
- $ie (nx) = 670$
- $je (ny) = 600$
- $lon(0,0) = 10^\circ, lat(0,0) = 47^\circ$

In the vertical, the model uses 60 layers extending from the surface to the lower stratosphere at approximately 24km. The simulation covers the whole year 2015.

This Berlin domain, nested within the European domain, is shown in Figure 1.

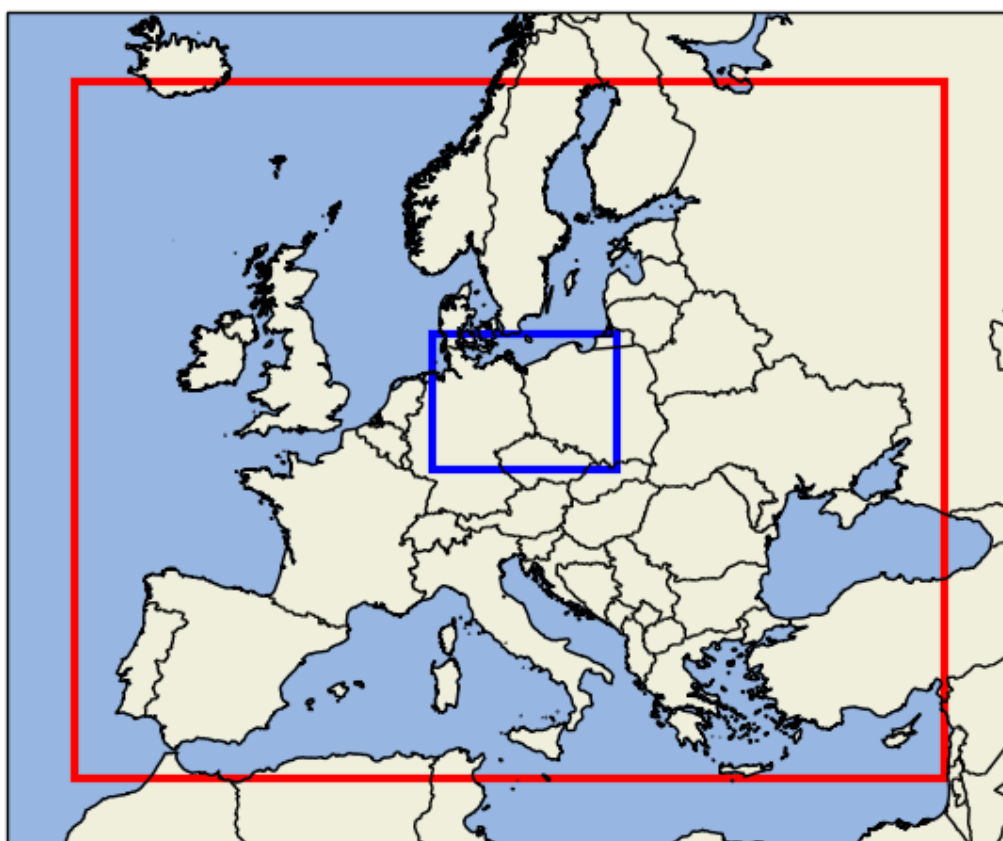


Figure 1: European domain (in red) and the nested Berlin domain (in blue).

3.1.2 LOTOS-EUROS

LOTOS-EUROS is an offline regional-scale Eulerian chemistry-transport model of intermediate complexity, developed in the Netherlands. It was originally developed for ozone and sulphur dioxide air pollution but was extended to cover other gases and aerosols in a bulk approach (fine and coarse mode aerosol). Gas-phase chemistry is a condensed version of the carbon bond mechanism CBM-IV (Gery et al., 1989). For aerosols ISORROPIA II (Fountoukis and Nenes, 2007) is used. The original approach with a mixing layer and reservoir layers in the lower troposphere was modified to efficiently use the input meteorology, to increase the vertical extent, and to be able to run on a higher horizontal resolution. Anthropogenic emissions are taken from an inventory, but emissions from sea salt, mineral dust and biogenic volatile organic compounds (VOC) are calculated online. Model output consists of hourly concentration and deposition fields; for the purpose of the

project, also optical properties have been put out. Details can be found in Manders et al. (2017).

The simulations of LOTOS-EUROS were driven by hourly meteorological output fields from the high-resolution COSMO-GHG run described above. The horizontal grid is identical to the COSMO-GHG grid, except that at 3 sides (north, west, and south) 4 grid cells are omitted to accommodate the boundary conditions, while at the east side 12 grid cells had to be omitted since the domain used by the WRF-VPRM model is slightly smaller than the COSMO-GHG at this side. While the horizontal resolution is identical to COSMO-GHG, the vertical resolution is reduced to 14 layers covering the lower 10 km based on COSMO's layer structure (lowest layer, combining next two layers, and combining each three layers going upwards). To support simulation of satellite retrievals, another 7 layers are added that are filled with concentrations from the global boundary condition models (C-IFS and GHG-IFS). Due to the high computational cost of full chemistry simulations, the LOTOS-EUROS runs cover only the months of February and July 2015.

3.2 Emissions

The simulations use the high-resolution emission dataset produced in the CHE project as described in Deliverable D2.3.

3.2.1 Anthropogenic emissions

This high-resolution anthropogenic emission inventory is described in Section 6 of Deliverable D2.3. It consists of the high-resolution (~1 x 1 km) domain of the TNO_GHGco inventory, merged with the emission inventory for the city of Berlin, provided by the "Senatsverwaltung für Stadtentwicklung und Umwelt" and processed for the simulations by Empa.

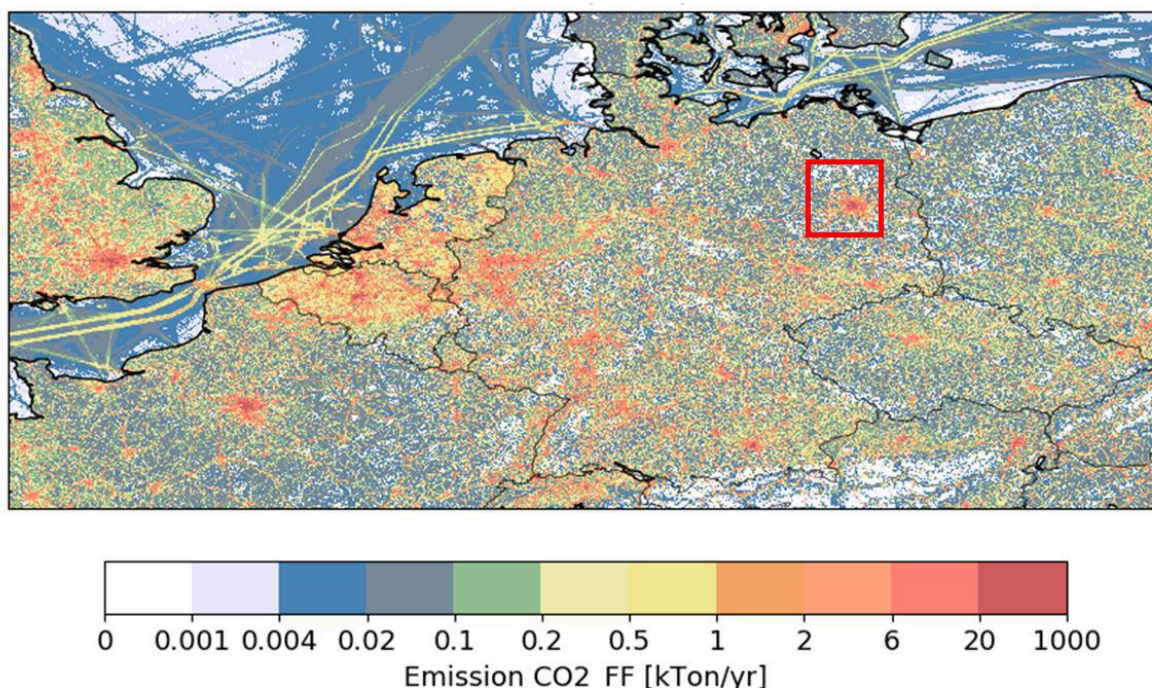


Figure 2: Domain of the TNO high resolution inventory at ~1 x 1km as prepared for CHE WP2. The Berlin inventory from the Senate Berlin is nested at the same resolution inside the red box.

The anthropogenic emissions are split by sector following the G-NFR (Gridding Nomenclature for Reporting) nomenclature.

Temporal profiles per category are provided with the emission inventory and applied in the models. Emissions from point sources are distributed vertically according to prescribed profiles, whereas all other emissions are released at the surface.

3.2.2 Biogenic emissions

The high-resolution biogenic emission inventory is described in Section 3 of Deliverable D2.3. It is computed with the VPRM model (Vegetation Photosynthesis and Respiration Model), a simple light-use-efficiency model driven by a combination of satellite reflectances from MODIS and meteorological input data. It is produced on the same grid as the anthropogenic emissions with a resolution of ~1 x 1 km.

3.3 Meteorological inputs

The Berlin simulations are nested inside the European simulations and use their results as boundary conditions for the meteorology and the tracers.

The COSMO-GHG model produces hourly meteorological fields that are used in the offline model LOTOS-EUROS to drive the transport of the chemical species.

3.4 Model outputs

The model outputs from the Berlin simulations are listed hereafter. They are provided as hourly data on the native model grids.

3.4.1 3D meteorology (COSMO-GHG)

Table 1: List of 3D meteorological outputs of the European simulation

Variable name	Variable abbreviation
Specific humidity	Q
Temperature	T
Pressure	P
Wind components	U,V
Cloud liquid water content	CLWC
Cloud ice water content	CIWC
Cloud cover	CLC

3.4.2 2D meteorology (COSMO-GHG)

Table 2: List of 2D meteorological outputs of the European simulation

- Cloud and precipitation: convective and large-scale precipitation, total cloud cover, cloud optical thickness
- Diagnosed planetary boundary layer height, soil moisture (multiple layers), snow depth
- Radiation: short- and long-wave radiation at ground, all components (up- and down) separately
- Surface fluxes: Sensible and latent heat fluxes

3.4.3 3D chemically passive tracers (COSMO-GHG and LOTOS-EUROS)

Table 3: List of output chemically passive tracers

Tracer name	Description
CO2_ALL	CO ₂ using all TNO emissions
CO_ALL	CO using all TNO emissions
CH4_ALL	CH ₄ using all TNO emissions
CO2_BG	CO ₂ from boundary condition
CO_BG	CO from boundary condition
CH4_BG	CH ₄ from boundary condition
CO2_GPP	CO ₂ from vegetation: Gross Photosynthetic Production (GPP)
CO2_RA	CO ₂ from vegetation: Respiration (RA)
CO2_A	CO ₂ using emissions from TNO for public power stations (GNFR A)
CO_A	CO using emissions from TNO for public power stations (GNFR A)
CO2_B	CO ₂ using emissions from TNO for industry (GNFR B)
CO_B	CO using emissions from TNO for industry (GNFR B)
CO2_C	CO ₂ using emissions from TNO for OtherStationaryComb (GNFR C)
CO_C	CO using emissions from TNO for OtherStationaryComb (GNFR C)
CO2_F	CO ₂ using emissions from TNO for road transport (GNFR F*)
CO_F	CO using emissions from TNO for road transport (GNFR F*)
CO2_O	CO ₂ using emissions from TNO for others (GNFR D,E,G,H,I,J,K,L)
CO_O	CO using emissions from TNO for others (GNFR D,E,G,H,I,J,K,L)

3.4.4 3D chemistry (LOTOS-EUROS)

LOTOS-EUROS including a full chemistry module, it produces 3D output fields for several trace gases. These fields, combined with the aerosols, are necessary for the study of the impact of aerosols on satellite retrievals.

- O₃
- NO₂
- NO
- NH₃
- SO₂
- HNO₃
- CO
- N₂O₅
- HCHO
- Isoprene
- PAN
- NMVOC (Total non-methane volatile organic compounds)

3.4.5 3D aerosols (LOTOS-EUROS)

Fine mode (PM_{2.5}):

- sea salt
- dust
- Elemental carbon (EC)
- Primary particulate matter (PPM)
- Primary organic matter (POM)
- SO₄
- NO₃
- NH₄

Coarse mode (2.5-10 µm):

- sea salt
- dust
- Elemental carbon (EC)
- Primary particulate matter (PPM)
- Primary organic matter (POM)
- SO₄
- NO₃

3D fields with optical properties of aerosol mixture at different wave lengths (440 nm, 550 nm, 765 nm, 870 nm, 1250 nm, 1600 nm, 1650 nm, 1950 nm, 2060 nm, 2350 nm):

- Aerosol optical depth (AOD), also provided as 2D total;
- Ångström parameter;
- number densities for fine and coarse mode;
- volume densities for fine and coarse mode;
- refractive indices for fine and coarse mode (REFR);
- single scattering albedo (SSA);
- asymmetry parameter (ASY).

3.4.6 2D fields (All)

XCO₂, XCH₄ and TC for all simulated 3D tracers.

4 Analysis of model outputs

One of the requirements of a Monitoring and Verification System is to be able to detect hotspots such as megacities or power plants and monitor their emissions. Such an emission estimate may rely on inversion methods combining satellite observations with numerical modelling of the transport of CO₂ from these sources. The resolution of such a modelling system should, ideally, be compliant with the resolution of the satellite observations of about 2 km x 2 km. A lower resolution may affect the quality of the estimates and the reliability of the inversion. It could lead to difficulties in localising and following the plumes. For instance, at coarse resolution, plumes from multiple point sources could mix and become indistinguishable. Moreover, small-scale flow phenomena e.g. due to topography or land-sea contrasts could be more difficult to simulate in a coarse resolution simulation. We will illustrate these issues with results of simulations by the COSMO-GHG model at 1 km and 5 km resolution, as well as results from the CAMS model at 9 km resolution. We focus on a smaller area centred on the power plant of Jänschwalde. This is one emission hotspot that can be targeted by the future Monitoring and Verification System (Kuhlmann et al. 2019). Its

plume is often mixed with the neighbouring power plants of Boxberg and Schwarze Pumpe (Figure 3).



Figure 3: Location of the Jänschwalde, Boxberg and Schwarze Pumpe power plants within the Berlin domain. In blue is the domain displayed in the following figures.

Figure 4 shows the total column CO₂ (XCO₂) on 9th March 2015 at 7:00 as simulated at 1 km and 5 km resolution, respectively. The direction and extent of the plume emanating from the power plant Jänschwalde is better represented in the high-resolution simulation. Moreover, the plume of Boxberg is split in two in the high-resolution simulation due to vertical shear in the horizontal winds between the planetary boundary layer and the free troposphere above.

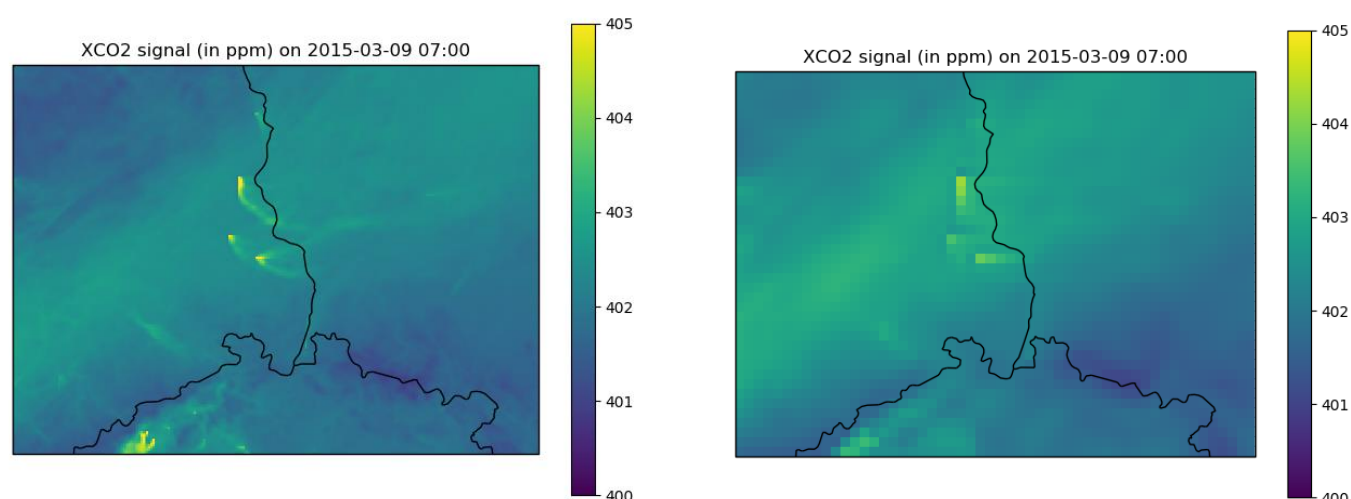


Figure 4: XCO₂ for the Berlin simulation (left, 1km resolution) and for the European simulation (right, 5km resolution) on 9th March 2015 at 07:00

Two hours later, the plumes have evolved and the plume of Jänschwalde is mixed with the ones of the other power plants in the low-resolution simulation while it is still clearly distinguishable in the high-resolution simulation (Figure 6). Moreover, the plume is less quickly diluted by numerical diffusion and is better visible with a peak amplitude of about 8 ppm above background as compared to only 5 ppm in the coarser simulation. Knowing that the satellites will have a precision of about 0.5 ppm, resolving such spatially confined plume enhancements could be crucial. Simulating tagged tracers representing only a part of the total emissions and processes could be useful in this task. To illustrate this, Figure 5 shows the XCO₂ enhancement due to the emissions from the GNFR-A category only.

We can further compare these results to the Tier-1 simulations at around 9 km resolution (Figure 7, left). These simulations however use the EDGAR emission inventory at 0.1° resolution. The coarser resolution of the emission inventory affects the simulated plume. For a start, the plume from Schwarze Pumpe seems to be absent from the inventory. Moreover, the CO₂ is emitted at the ground level, which leads to a different direction of the plume at that time, going north-west instead of south-west. The magnitude of the plume in the Tier-1 simulation is also smaller than the 5 km resolution simulation using the same emission inventory (Figure 7, right). This could be due to weaker winds leading to more accumulation in the 5 km resolution or to the fact that the low resolution dilutes the emissions over several larger grid points, thus reducing the signal. The seemingly stronger background value in the 5 km simulation is likely due to the different biogenic emission inventory used in comparison to the Tier-1 simulation.

A more thorough and quantitative analysis of the results, including comparison with the Tier-2 runs as well as LOTOS-EUROS simulations will be performed as soon as all the data will be available.

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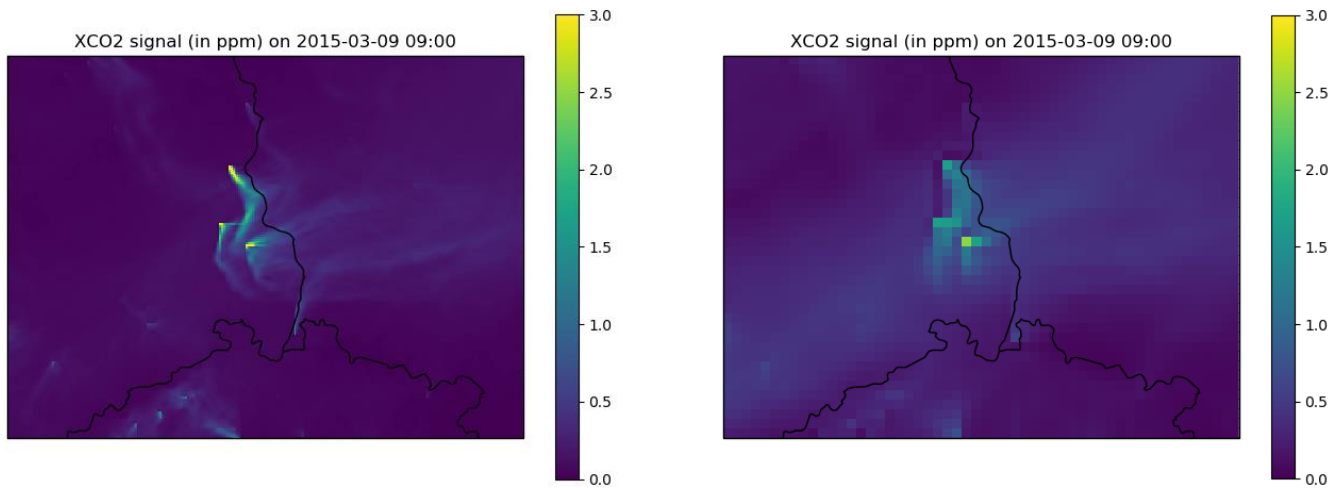


Figure 5: XCO₂ from the GNFR-A category (public power stations) for the Berlin simulation (left, 1km resolution) and for the European simulation (right, 5km resolution) on 9th March 2015 at 9:00

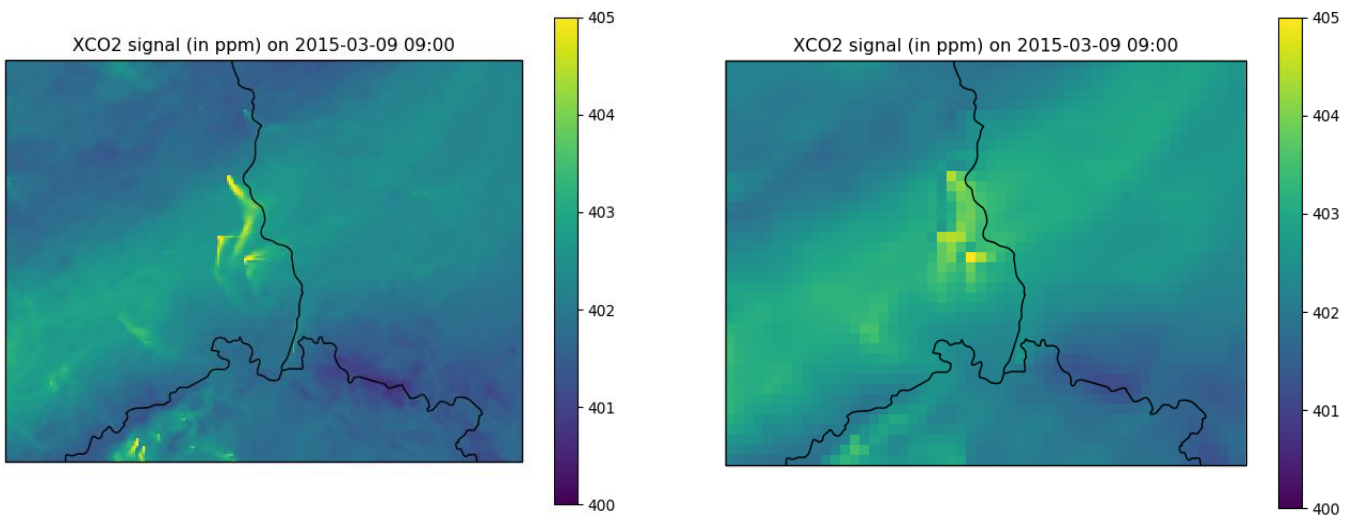


Figure 6: XCO₂ for the Berlin simulation (left, 1km resolution) and for the European simulation (right, 5km resolution) on 9th March 2015 at 9:00

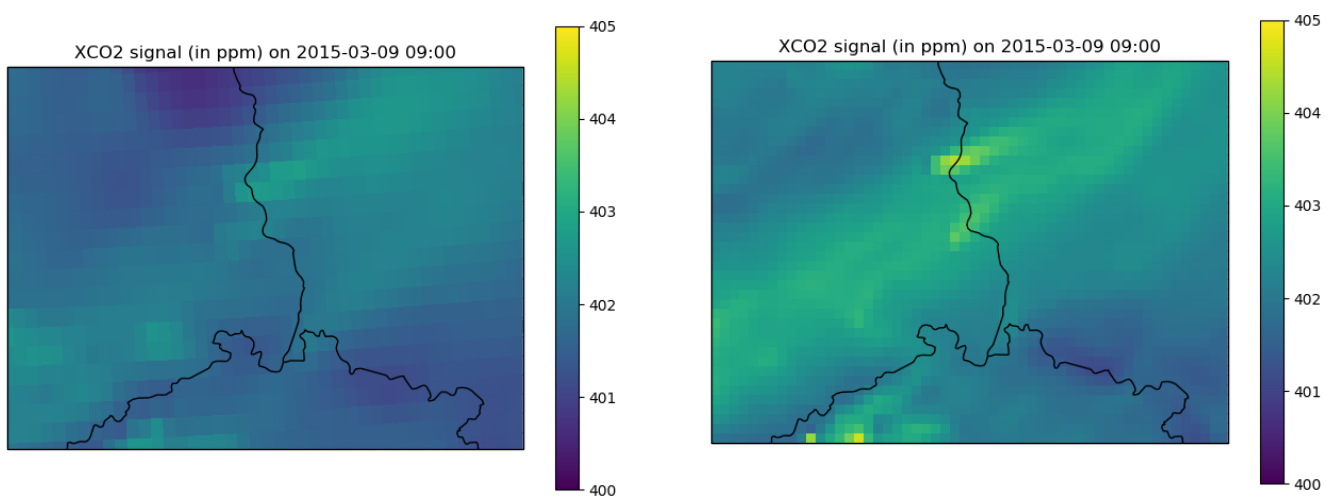


Figure 7: XCO₂ for the Tier-1 simulation (left, 9km resolution, EDGAR inventory) and for the European simulation (right, 5km resolution, EDGAR inventory) on 9th March 2015 at 9:00

5 Status of simulations and deliverables, delays, plan for completion

5.1 European simulations

The simulations covering the European domain for the year 2015 and 2030 have been completed by all three of the modelling groups, namely Empa using COSMO-GHG, MPI using WRG-GHG and TNO using LOTOS-EUROS.

The full 3D fields have been uploaded to the ECMWF tape archive and are available for download.

The deliverable describing the setup of these simulations and presenting their result is in the hand of MPI and close to completion.

5.2 Berlin simulations

The simulations covering the Berlin domain described in this deliverable are fully completed. The results are available upon request to the authors.

SRON is also producing simulations with WRF-CHEM over Berlin, to study the impact of aerosols on satellite retrievals. These simulations are related to the task 2.5 and the Deliverable D2.7 which is due in month 39. Some first results have already been produced for testing but the definitive dataset will be provided at a later time.

5.3 Beijing simulations

The setup for these simulations was discussed between TNO (using LOTOS-EUROS) and SRON (using WRF-Chem). The current plan is to simulate not only Beijing but also Shanghai (for its contrasting conditions) using a separate domain. Suitable months have been selected in winter and summer, with spells of high pressure / clear sky conditions. WRF-Chem output is currently being generated for these domains and time windows, which will be passed on - once finalized - to TNO as driving meteorological fields for LOTOS-EUROS simulations.

These simulations are produced to study the impact of aerosols on satellite retrievals and are related to the Task 2.5 and the Deliverable D2.7 which is due in month 39. They will therefore be provided at a later time.

5.4 Connections to WP5

The task 5.2 of the CHE WP5 focuses on the requirements for CO₂ Emission and Transport Models in a Monitoring and Verification System. It provides a link between the library of simulations of the WP2 and the other WP and synthesizes the results in terms of recommendations for a pre-operational emission estimation system. As such, a joint WP2-WP5 workshop will be organised at Empa in May 2020 to further discuss the results of WP2 and how it translates into clear recommendations for WP5.

6 Conclusion

The WP2 was tasked to produce a library of simulations covering multiple models and multiple scales, from the global scale down to the regional scale. With the completion of the Berlin simulations, the library of simulations is finalized. It will allow for a quantitative analysis of the modelling requirements necessary to support the satellite constellation observing CO₂. The initial analysis of the results hints at a need of high-resolution simulations in order to be able to localize and follow hotspot emissions above the background fields. Later, with the help of OSSEs, a more precise and quantitative assessment of the benefits of high resolution will shed light on the modelling needs of the pre-operational real-time hotspot emission estimation system which is planned in 2021.

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LOGOFLUX-2, Final report of CarbonSat Earth Explorer 8 Candidate Mission “LOGOFLUX 2– Flux Inversion Performance Study”, NOVELTIS, version 1.1, 12 October 2015.

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