CoCO2

Prototype system for a Copernicus CO_2 service

Definition of simulation cases and model system for building a library of plumes

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coco2-project.eu

Co-ordinated by ECMWF

D4.1 Definition of simulation cases and model system for building a library of plumes

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1 Executive Summary

This document provides a description of detailed benchmark simulations. These simulations are planned in support of the development and application of high-resolution atmospheric transport and inversion systems. These systems cover limited geographical areas and address scales from mesoscale weather phenomena to individual plumes as they are resolved by CO2M. Specifically, we propose to simulate four stacks from large facilities in Europe, Russia, and South Africa. Additionally, simulations are proposed for the cities of Berlin and Paris, and the “Randstad” region in the Netherlands. For all these simulation cases, surface and/or satellite observations are available to evaluate the simulations. Two simulation protocols (Bełchatów and Jänschwalde power stations) closely follow the simulation protocol previously used in the CoMet project. The Berlin case builds on a recent paper by Klausner et al. (2020). Two other cases (Lipetsk in Russia, and Matimba in South Africa) focus on detection of stack plumes from space (see e.g. Hakkarainen et al. (2021)). For the stack cases, the effects of atmospheric chemistry (e.g. lifetime NO_x) will be explicitely considered.

The document further provides brief descriptions of the simulation set-up and the participating models.

2 Introduction

2.1 Background

Monitoring emissions critically depends on addressing the local and national scales. The analysis and developments in WP4 will rely on state-of-the-art transport models and inversion approaches. However, these systems require improvements in their efficiency and robustness to ensure that they can be applied operationally.

The future CO2M satellites will be able to identify the plumes of strong point sources and clusters of sources (e.g. cities, industrial complexes) with a horizontal resolution of 2 km x 2 km. In order to use this information in atmospheric inversion systems, the underlying atmospheric transport models should be able to resolve the plumes and reproduce their basic properties. Currently, large uncertainties exist regarding the ability of atmospheric transport models to describe individual observed plumes. Moreover, simulation results are sensitive to different model settings such as resolution, boundary layer and advection schemes, and to the representation of the source such as its temporal variability and injection height in the case of stack emissions. Moreover, models that run on regional scale, are also sensitive to meteorological forcing.

In order to test the current high-resolution transport models, this document proposes several test cases that are relevant for emission verification. These cases are meant as benchmark cases that are simulated by an ensemble of high-resolution models (10 m – 1 km). The simulations will not only include CO_2, but also co-emitted species like NO_2 and CO, simulated with full or simplified linear chemistry. Cases will be presented for which suitable validation data (satellite, ground-based, (aircraft) campaigns) is available.

The case studies will be conducted in close connection with WP3, in which the global system is developed. One option is to embed regional models in this global system to provide more accurate regional estimates. Also, the use of satellite data to observe plumes through their NO_2 and/or CO atmospheric imprint will receive special attention. Current satellites like TROPOMI observe emission plumes from space, and the use of this information to infer information about CO_2 emissions is deemed very important.

2.2 Scope of this deliverable

2.2.1 Objectives of this deliverables

The main objective of this report is to document the case studies, the participating model systems, and available observational datasets to evaluate the simulations.

2.2.2 Work performed in this deliverable

This deliverable marks the start of the simulations, based on the cases defined in this report. The work performed involved (1) collecting a list of proposed cases on existing and new efforts in the community (2) preparing descriptions of the participating models (3) collecting information about the cases and defining simulation periods based on the availability of observational data. The work has been mostly performed by WUR, but with the help of the participating modellers. Moreover, use was made of existing simulation protocols (e.g. the CoMet project).

2.2.3 Deviations and counter measures

None

3 Case Studies

3.1 Overview

Table 1 provides an overview of the cases and the expected simulation period. These cases were selected based on the availability of observations, and range from simulations of isolated plumes to simulations of complex clusters of sources in urban areas.

Table 1: List of case studies and simulation period

Case ID	Description	Time Period
BEL	Power plant Bełchatów, Poland	6 + 7 June 2018
JAE	Power plant Jänschwalde, Germany	22 + 23 May 2018
LIP	Steel plant Lipetsk, Russia	13 June 2019
MAT	Power plant Matimba, South Africa	25 July 2020
PAR	Paris Urban Area, France	Jan, Mar, Aug 2018
NL	Randstad area, Netherlands	21-02-2018 to 27-02-2018 29-06-2018 to 05-07-2018
BER	Berlin urban area, Germany	18-27 July 2018

3.2 Details of the case studies

3.2.1 General notes on the stack cases

The setup for the Bełchatów and Jänschwalde power stations closely follows the CoMet simulation protocol (Brunner, 2020), including the choice of the simulation periods. For all sites, the emissions are provided for the individual stack locations (or in the case of Jänschwalde; the location of groups of stacks), and a central location which is representative for the entire plant. All participants should include a single CO_2 tracer and emission for the central location *("center").* Participants with high resolution models may optionally include a second CO_2 tracer which is emitted from the individual locations and include plume rise. Models that simulate chemistry should also emit CO, NO_x and hydrocarbons from the plume. The proposed emission height and vertical extent has been calculated using a plume rise model, using typical stack properties from Pregger & Friedrich (2009).

Models need initialization and boundary conditions. Boundary conditions from CAMS/IFS (chemistry) and ERA5 (meteorology) will be provided for the test cases.

3.2.2 Bełchatów (BEL)

The Bełchatów Power Station is a coal-fired power station near Bełchatów, in central Poland. Emissions are released from two 299 m high stacks.

The emission details for the simulations are provided in Table 2. The CO_2 emissions are based on the CoMet protocol. For the chemistry simulations, the CO and NO_x emissions are obtained from the European Pollutant Release and Transfer Register (E-PRTR), based on data from 2018. Other hydrocarbon emission data can also be found there. The simulation period spans from 06-06-2018 00:00 UTC to 08-06-2018 00:00 UTC.

Observations are available from the CoMet measurement campaign, which includes both aircraft in-situ observations (including CO_2, CO, NO_2, and meteorological variables like temperature, humidity, pressure, and wind speed), and remote sensing observations (CO_2, XCO_2). The observations, from three different aircraft, are available for 07-06-2018, between 12:20 UTC and 15:20 UTC. In addition, TROPOMI satellite observations will be used for validation.

Table 2: Emission details Bełchatów case

	Coordinates (longitude, latitude)	*Emission CO_2 (kg CO_2/s)*	*Emission CO (kg CO/s)*	*Emission NOx (kg NO_2/s)*
Center	19.3261°E, 51.2660°N	1217.7	0.8334	0.9538
East[1]	19.3285°E, 51.2660°N	608.8	0.4167	0.4769
West[1]	19.3237°E, 51.2660°N	608.8	0.4167	0.4769

[1] High-resolution models can emit an extra tracer at exact locations

3.2.3 Jänschwalde (JAE)

The Jänschwalde Power Station is a coal-fired power station near Cottbus, close to the German-Polish border. The Jänschwalde power station has 9 cooling towers (120 m high) in groups of three, of which only two towers per group are active. Following the CoMet simulation protocol, each group is treated as a single source location.

The emission details are provided in Table 3. The CO_2 emissions are based on the CoMet protocol. For chemistry simulations, the CO and NO_x emissions are obtained from the E-

PRTR, based on data from 2017. The simulation period spans from 22-05-2018 00:00 UTC to 24-05-2018 00:00 UTC.

Observations are available from the CoMet measurement campaign, similar to the observations from the Bełchatów case, only excluding CO and NO_2 observations. The observations are available for 23-05-2018, between 06:29 and 11:34 UTC. In addition, TROPOMI satellite observations will be used for validation.

Table 3: Emission details Jänschwalde case

	Coordinates (longitude, latitude)	*Emission CO_2 (kg CO_2/s)*	*Emission CO (kg CO/s)*	*Emission NOx (kg NO2/s)*
Center	14.4580°E, 51.8361°N	732.5	0.3422	0.6021
East[1]	14.4622°E, 51.8360°N	244.2	0.1141	0.2007
Center[1]	14.4580°E, 51.8361°N	244.2	0.1141	0.2007
West[1]	14.4538°E, 51.8362°N	244.2	0.1141	0.2007

[1]Optional for a second CO_2 scalar

3.2.4 Lipetsk (LIP)

This steel plant is owned by NLMK Group. They claim to be the largest steelmaker in Russia and one of the most efficient in the world. This case was provided by Manu Goudar Vishwanathappa from SRON, who detected a CO plume from TROPOMI (June 13, 2019). The plume is also visible in TROPOMI NO_2 (see Figure 1).

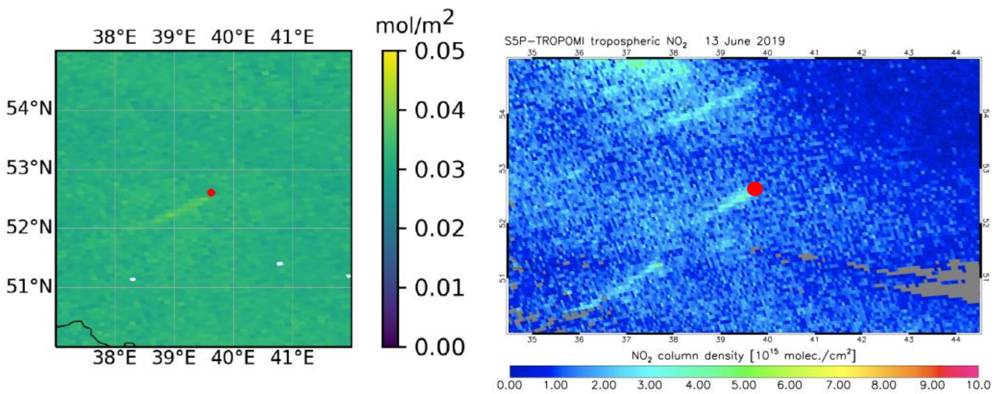


Figure 1: TROPOMI satellite images collected on June 13, 2019. Left: CO, right: NO_2. The red dot denotes the location of the steel plant.

The emission details are provided in Table 4. The emissions are obtained from the 2019 annual report of the NLMK group[1]. The simulation period spans from 13-06-2019 00:00 UTC to 14-06-2019 00:00 UTC.

[1] https://nlmk.com/en/ir/reporting-center/annual-reports/

Table 4: Emission details Lipetsk case

	Coordinates (longitude, latitude)	*Emission CO_2 (kg CO_2/s)*	*Emission CO (kg CO/s)*	*Emission NOx (kg NO_2/s)*
Center	39.6196°E, 52.5603°N	*1014.0*	7.4562	0.8302

3.2.5 Matimba (MAT)

The Matimba power station is a dry cooled, coal-fired power plant in the north-east of South Africa, approximately 300 km north of Johannesburg. The power plant has two 250 m high stacks. This case is based on Hakkarainen et al. (2021). Emissions and location are given in Table 5.

The emissions for the simulations are based on reported CO_2, CO, and NO_x emissions[2], averaged the entire year 2018. The simulation period spans from 25-07-2020 00:00 UTC to 26-07-2020 00:00 UTC.

CO_2 observations are available from OCO-2, NO_2 observations from TROPOMI (Hakkarainen et al., 2021).

Table 5: Emission details Matimba case.

	Coordinates (longitude, latitude)	*Emission CO_2 (kg CO_2/s)*	*Emission CO (kg CO/s)*	*Emission NOx (kg NO_2/s)*
Center	27.6109°E, 23.6688°S	*954.2*	0.3567	2.4920
North[1]	27.6106°E, 23.6676°S	*477.1*	0.1784	1.2460
South[1]	27.6112°E, 23.6699°S	*477.1*	0.1784	1.2460

[1]Optional for a second CO_2 scalar

3.2.6 Paris (PAR)

The Paris urban area, centred on the city of Paris, is a dense urban area. It is the fourth in Europe in terms of population, with nearly 6 million inhabitants in its core part gathering the city of Paris and the "petit couronne" and ~10 million inhabitants in total (numbers can vary significantly depending on the definition given to the different areas). Annual CO_2 Emissions from the core part of the urban area exceed 20 $MtCO_2.yr^{-1}$. Its distance from other major CO_2 sources, and the relatively flat topography around this area in addition to its high level of emissions concentrated over a relatively small surface makes it a prominently favourable test case for plume modelling and inversions. LSCE has been setting CO_2 atmospheric *in situ* measurement and inverse modelling frameworks to monitor the emissions from this urban

[2] https://www.eskom.co.za/Whatweredoing/AirQuality/Pages/Matimba-Power-Station.aspx

area since 2010. Estimates of the Paris CO_2 emissions from these frameworks have been documented in Bréon et al. (2015) and Staufer et al. (2016).

LSCE and the company Suez-Origins currently collaborate for such an activity with the maintenance of 7 stations with in situ high precision CO_2 and CO sensors around and within the core area, the deployment of lower cost CO_2 sensors across this area, and routine CO_2 simulations and inversions based on the WRF-Chem modelling configuration of Lian et al. (2019) and Lian et al. (2020) (see 4.1.2), on an update of the inverse modelling frameworks of the series of studies Bréon et al. (2015), Staufer et al. (2016) and Wu et al. (2016) and a 1-km resolution inventory compiled by Suez-Origins. This activity will be supported by the PAUL Horizon 2020 Green Deal project. The observation network is complemented by a TCCON site within Paris[3] . Clear images of the NO_2 plume from Paris have been provided by TROPOMI (Lorente et al., 2019).

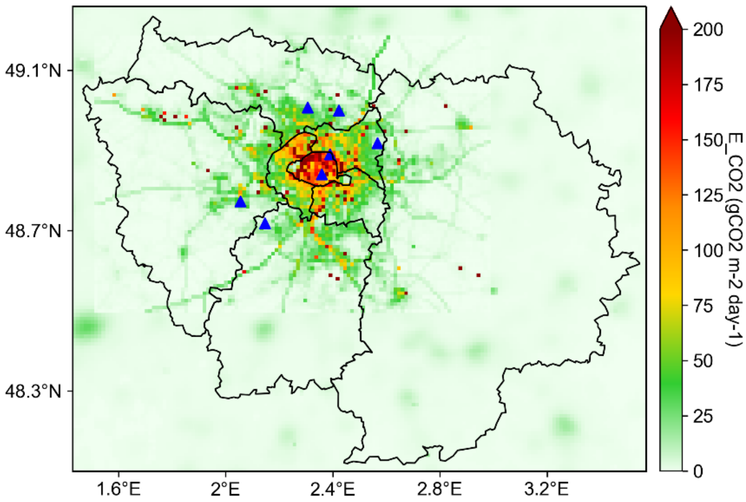


Figure 2: Distributions of the CO_2 emissions in the region of Paris (Île-de-France) for a typical weekday in November from the Suez-Origins inventory (complemented by the ODIAC inventory for the Eastern and Southern borders of the area), together with the location of seven CO_2 high-precision measurement stations as well as the administrative limits and partition of the region (the city of Paris is at the centre). The core of the urban area roughly corresponds to the four administrative units at the core of this region.

Simulations for this megacity will focus on few days in January and March 2018, including two time-windows when TROPOMI measured NO_2 with a zooming mode (at 2.4 x 1.8 km^2 resolution) during the first week of March, and in August 2018 (to have simulations both in winter and summer).

The location of the CO_2 / CO stations that will be used for the validation is provided together with a map of the CO_2 emissions in the Paris area (based on the Suez Origin inventory) in Figure 2. The Paris TCCON site is co-located with one of the two stations within the city of Paris (the southern one). The NO_2 images from TROPOMI will be used to assess the position, extent and shape of the XCO2 plume simulations. The data from the dense regional air quality network and the NO_2 concentrations from TROPOMI as such could also be considered in the course of the project if simulations of pollutants are conducted.

3.2.7 Randstad (NL)

The Randstad is a conurbation in the western part of the Netherlands, which includes the four largest Dutch cities: Amsterdam, Rotterdam, The Hague, and Utrecht. The area houses roughly half of the Dutch population. In addition to the Schiphol and Rotterdam The Hague airports, the Randstad contains the Port of Rotterdam, which is the largest seaport in Europe.

[3] https://tccon-wiki.caltech.edu/Main/Paris

Both Schiphol airport and the Port of Rotterdam are areas with some of the highest CO_2 emissions in the Netherlands.

The simulations over the Randstad will focus on two one-week periods: one during the summer (29-06-2018 00:00 UTC to 06-07-2018 00:00 UTC) and winter (21-02-2018 00:00 UTC to 28-02-2018 00:00 UTC). The simulations will be performed with both LOTOS-EUROS and DALES. More information on the model setup and e.g. emission inventories is provided in Section 4.1.6.

For the validation, CO_2 observations are available at several locations:

- Cabauw (KNMI, ICOS, 51.97N, 4.93E): CO_2 concentrations and fluxes along a 213m tall tower.
- Loobos (WUR, ICOS, 52.17N, 5.74E): CO_2 concentrations and fluxes along the 24 m tall tower.
- Veenkampen (WUR, 51.98N, 5.62E): Near surface CO_2 concentrations and fluxes.

Other air quality observations are available from the National Institute for Public Health and the Environment (RIVM), which contains (among others) observations of CO, NO, NO_2, and O_3 at approximately 40 locations in the Randstad.

3.2.8 Berlin (BER)

This study case will be based on Klausner et al. (2020). The time period for which aircraft observations of greenhouse gas concentrations & reactive gases (NO_2, O_3, CO) are available (18-27 July 2018) as indicated in Figure 3. Additionally, TROPOMI satellite observations will be used to validate the models.

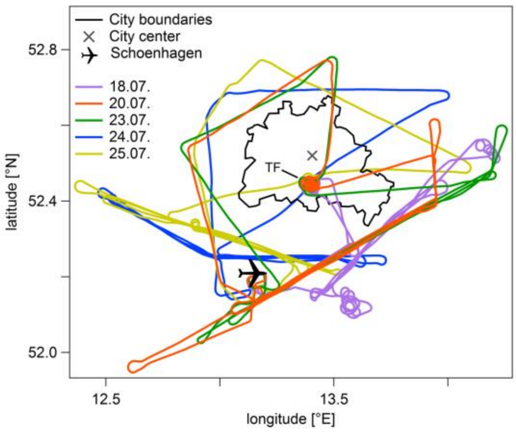


Figure 3: From Klausner et al. (2020): Flight paths of the DLR Cessna.

4 Model Systems

In total, 7 different models will participate in the simulations of the 7 different cases, as summarized in Table 6.

Table 6: Participating models

	BEL	*JAE*	*LIP*	*MAT*	*PAR*	*NL*	*BER*
COSMO-GHG	O	O	O	O			O
WRF-CHEM					O		
ICON-ART		O					
LOTOS-EUROS	O	O				O	O
WRF-GHG							
DALES						O	
MicroHH	O	O	O	O			

4.1 Details model systems

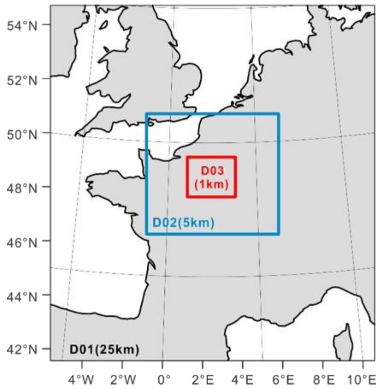
4.1.1 COSMO-GHG

The COSMO model for non-hydrostatic limited area modelling was developed within the context of the Consortium for Small-Scale Modelling, a consortium of seven European national weather services. COSMO-GHG is an extension of COSMO with modules for the passive transport of greenhouse gas (GHG; Liu et al., 2017), built on top of the tracer module for COSMO (Roches and Fuhrer, 2012). 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). For the simulations carried out in CoCO2, the GPU-accelerated version of COSMO 5.09 (COSMO 6, if available) will be applied on a 1x1 km^2 grid.

COSMO can be obtained freely for research purposes, after accepting the license at https://www.cosmo-model.org/content/consortium/licencing.htm. For access to COSMO-GHG, Empa may be contacted.

4.1.2 WRF-CHEM

WRF-Chem (Grell et al. 2005) is a widely used regional scale meteorological-chemistry transport coupled model. The WRF-Chem V3.9.1 simulations of the CO2 plume from Paris are conducted in collaboration between LSCE and Suez-Origins. The configuration of the model for these simulations is that documented and evaluated in Lian et al. (2018), Lian et al. (2019) and Lian et al. (2020), retaining the reference parameterization of Lian et al. (2020). This configuration is based on 3 nested domains (see Figure 4) whose respective horizontal resolution is 25, 5 and 1 km. The innermost domain covers the whole Paris urban area.



Domain	Number of grid cell (lon * lat)	Coordinates (lon * lat)
D01	55 * 60	-7.76°W~12.76°E, 41.69~55.01°N
D02	111 * 101	-1.39°W~6.39°E, 46.55 ~51.06°N
D03 (innermost)	201 * 166	1.05 °E~3.81°E, 47.98~49.46°N

Figure 4: WRF-Chem configuration: coverage and spatial resolution of the different domains

WRF-Chem is fed with the 1-km resolution Suez Origins inventory of the CO_2 anthropogenic emissions of the Paris urban area complemented by the ODIAC global inventory for the year 2018 (version ODIAC2020; Oda and Maksyutov, 2011) at 1 km resolution for the emissions outside this area. The WRF-Chem configuration used here includes the VPRM model (Ahmadov et al., 2007) for the computation of the CO2 land ecosystem fluxes. At the boundary of the outermost domain, the simulation is forced with the CO2 fields from the CAMS analysis (version v18r1, Chevallier, 2018[4]). The simulations keep track of the specific signature of part of these fluxes (like that of biogenic and anthropogenic fluxes in each domain) along with the variations of the full 3D-field of total CO2. In particular it tracks that of the emissions from the core of the urban area, which should correspond to the plume from the Paris area as it can be seen in XCO2 spaceborne images (see Figure 5).

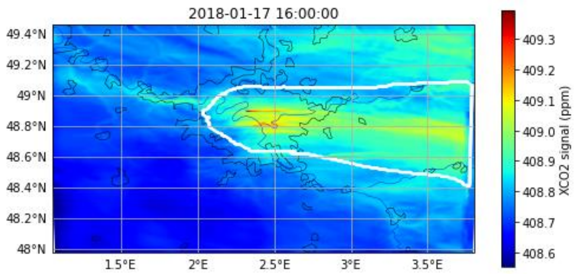


Figure 5: Simulation of the XCO2 field in the Paris area at 1 km resolution (in domain D03 of the WRF-Chem model). The white line delimits the signature of the emissions from the core part of the urban area

4.1.3 ICON-ART

ICON-ART (Aerosol and Reactive Trace gases) is an extension of ICON (ICOsahedral Nonhydrostatic model), developed to enable simulations of gases, aerosol particles and related feedbacks in the atmosphere (Rieger et al., 2015).

4.1.4 LOTOS-EUROS

LOTOS-EUROS is an offline regional-scale Eulerian chemistry-transport model that is used to simulate concentrations of trace gasses and aerosols in the boundary layer and free troposphere (Manders et al., 2017). The model domain is typically covering Europe at scales of 10-20 km, or a selected region with resolutions up to 1-2 km. Meteorological input is by default obtained from ECMWF, but could also be obtained from other sources. In the vertical, the model covers the troposphere using typically 12 layers that are formed as a coarsening of the meteorological input. Gas-phase chemistry is a described using a carbon bond mechanism. Formation of secondary inorganic aerosol is described using ISORROPIA-II.

[4] https://apps.ecmwf.int/datasets/data/cams-ghg-inversions

Anthropogenic emissions are taken from an inventory, but emissions from sea salt, mineral dust and biogenic volatile organic compounds (VOC) are calculated online.

In this project, the model will use meteorological data from COSMO-GHG when possible, and in this case the horizontal grid will also be taken from this model; otherwise, ECMWF data will be used. The simulations will provide concentrations of trace gases and aerosol, as well as selected chemical productions and loss rates; these could then be used by models with a limited number of tracers to parameterize production and loss. Optical properties of the aerosols will also be put out to facilitate simulation of synthetic satellite observations.

4.1.5 WRF-GHG

WRF-GHG is an extension of the Weather Research and Forecast (WRF) model, developed to study the transport of greenhouse gases as passive tracers (Beck et al., 2011).

4.1.6 DALES

The Dutch Atmospheric Large Eddy Simulation model (DALES, Heus et al., 2010) is a large-eddy simulation code, developed by a consortium of Dutch universities. In the *Ruisdael Observatory* project, DALES is currently being extended so that it is suitable for running realistic LES on domains of ~100-200 km at 100 m resolution.

For the experiments over the Randstad, time varying CO_2 emissions from the Dutch emission registry will be used. These emissions are available at a 1 x 1 km^2 resolution and have been postprocessed to a 100 x 100 m^2 resolution using high resolution human activity data. An example is shown in Figure 6. In addition, point source emissions (including the relevant variables required to calculate plume rise) are available for the largest industrial facilities. Combined with the CHTESSEL based land surface model, which includes the A-Gs scheme to account for the vegetation assimilation and soil respiration of CO_2, it is possible to study both the anthropogenic sources and biogenic sources and sinks of CO_2. The model output will include the background, anthropogenic, and total CO_2 concentrations.

The model domain is equal to the area shown in Figure 6, and consists of 1728 x 1152 grid points in the horizontal, which – with a horizontal grid spacing of 100 m – results in a domain of 172.8 x 115.2 km^2.

DALES is open-source software, available at: https://github.com/dalesteam/dales

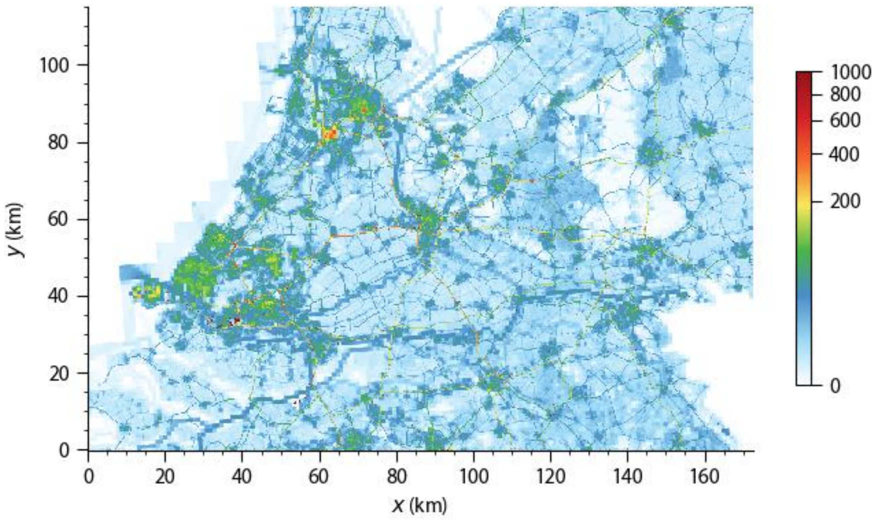


Figure 6: Example CO_2 emissions (in kg CO_2 / h) for the Randstad area, on 19-08-2017, 12:00 UTC

4.1.7 MicroHH

MicroHH is a direct numerical simulation (DNS) and large eddy simulation (LES) model, capable of running on both CPUs and GPUs, coded in C++/CUDA-C (Van Heerwaarden et al., 2017). The current version includes a basic emission module, which allows for stationary or moving, constant and/or time varying point or line sources for scalars. In addition, simplified chemistry can be added using the Kinetic Pre-Processor Software package. Within COCO2 we will streamline the chemistry with WP3 such that MicroHH can use boundary conditions from the IFS system, and "adds" an isolated plume. Focus will be on:

- Turbulent dispersion of plumes, depending on wind and atmospheric stability
- Chemical decay of NOx in the plume, depending on large-scale fields of e.g. ozone
- Possible effects of plume rise

MicroHH is open-source software, available at https://github.com/microhh/microhh and www.microhh.org

5 Simulation protocol

As outlined in the CoCO2 Data Management Plan, all model output will be made available in NetCDF-4 format, compliant with CF conventions. To simplify the comparison of different models, the NetCDF files should (as a minimum) include the variables and follow the conventions summarized in Table 7 and Table 8. Output frequency should be minimal 15 minutes.

Table 7: Overview NetCDF dimensions

Name	*Description*
longitude	Number of grid points in zonal direction
latitude	Number of grid points in meridional direction
level	Number of full (cell center) vertical levels
levelh	Number of half (cell edge) vertical levels
time	Number of time steps

Table 8: Overview NetCDF variables

Variable	*Description*	*Units*	*Dimensions*
time	Time	UTC	time
longitude	Zonal location	degrees	latitude, longitude
latitude	Meridional location	degrees	latitude, longitude
p	Air pressure at cell center	Pa	time, level, latitude, longitude
z	Height above surface at cell center	m	time, level, latitude, longitude
ph	Air pressure at cell edge	Pa	time, levelh, latitude, longitude
zh	Height above surface at cell edge	m	time, levelh, latitude, longitude
ta	Air temperature	K	time, level, latitude, longitude
hus	Specific humidity	$kg\ kg^{-1}$	time, level, latitude, longitude
ua	Eastward wind	$m\ s^{-1}$	time, level, latitude, longitude
va	Northward wind	$m\ s^{-1}$	time, level, latitude, longitude
wa	Vertical velocity	$m\ s^{-1}$	time, level, latitude, longitude
co2	CO_2 dry air mole fraction	$mol\ mol^{-1}$	time, level, latitude, longitude
ps	Surface pressure	Pa	time, latitude, longitude
zsurf	Surface elevation	m	time, latitude, longitude
tracer	Chemical tracer mole fraction	$mol\ mol^{-1}$	time, level, latitude, longitude

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