Supplement S2

Protocol for CoMet Power Plant Plume Simulations

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1. Background and objectives

Power plants are a major source of CO_2 globally. Although CO_2 emissions are routinely monitored in many power plants, especially in developed countries, these numbers are usually not publicly available and a complete record of all emissions globally is still far from reality. An independent assessment of emissions from large point sources based on atmospheric observations is much needed and is a central goal of future satellite missions such as CO2M.

In May/June 2018, the CO_2 plumes of two large coal-fired power plants, Belchatow in Poland and Jänschwalde in Germany, were observed with aircraft in situ and remote sensing measurements in the context of the CoMet campaign. These measurements provide a unique opportunity to study the capability of atmospheric transport models to simulate such plumes in a realistic manner and to define optimal sampling and modelling strategies for emission quantification. Several research groups have already performed simulations using a range of different modelling techniques. After exchanging information on the individual activities during an online meetings, the groups agreed on a coordinated effort, where all groups conduct additional simulations in a harmonized setup and with well-defined model outputs supporting data analysis and comparison. This document describes the modelling protocol for this effort.

The overall aims of the study are:

- Evaluate the model simulations against in situ and remote sensing observations both with respect to meteorology and with respect to trace gas concentrations.
- Compare the model simulations against each other to compare the way the spatiotemporal variability and dispersion of the plumes is represented. This includes a comparison of the model simulations resampled to the resolution of future satellite missions.
- Analyse how well emissions can be quantified using different measurement strategies by sampling the simulated plumes at the locations of hypothetical observations (including slicing and mapping of the plumes by remote sensing instruments).
- Provide recommendations for future measurement campaigns.
- Demonstrate the potential & limitations of model simulations and provide recommendations for optimal model setups.

2. Simulations

Since the protocol should be applicable to a wide range of models with different resolutions and associated computational costs, the protocol defines a set of minimal and optimal requirements. Whenever affordable, the optimal setup should be selected, e.g. the longer simulation time periods defined in Table 1.

Table 1. Simulations

ID	Power plant	Domain lon range	 lat range	Time period (time in UTC, dates in 2018)	Mandatory
BEL_M	Belchatow	18.7–19.9°E	50.95–51.55°N	06/06 00:00 – 08/06 00:00	yes
BEL_O	Belchatow	18.7–19.9°E	50.95–51.55°N	28/05 00:00 – 08/06 00:00	no
JAE_M	Jänschwalde	13.8–15.0°E	51.50–52.10°N	22/05 00:00 – 24/05 00:00	yes
JAE_O	Jänschwalde	13.8–15.0°E	51.50–52.10°N	18/05 00:00 – 24/05 00:00	no

Each simulation needs to include the following minimum set of CO2 tracers:

CO2_PP_H: CO_2 emitted from power plant for high release case

CO2_PP_M: CO_2 emitted from power plant for middle release case (reference case)

CO2_PP_L: CO_2 emitted from power plant for surface release case

Models able to incorporate temporally changing vertical emission profiles should additionally include a tracer

CO2_PP_T: CO_2 emitted from power plant with temporally varying vertical profiles

See section 3.2 for details about emission heights derived from plume rise computations.

Additional CO_2 tracers (optional) should be denoted as follows:

CO2_BG: Background CO_2 transported from outside model domain

CO2_ANTH: CO_2 from anthropogenic emissions within model domain except for emissions from selected power plant

CO2_BIO: CO_2 from biospheric fluxes (photosynthesis and respiration). For online VPRM, parameters are specified in a common table

CO2_TOT_ANTH: Total CO_2 including background and all anthropogenic sources (including power plant) but not the biospheric signal.

If needed, simulations should include a spin-up prior to the starting dates listed in Table 1 so that any initialization effects do not compromise the results for the indicated period. The model domain can be larger than the minimum domain specified in Table 1. Simulations should be performed at a typical resolution of the model and on the model's specific projection. Output needs to be generated on, or projected to, a regular latitude-longitude grid (see section 4).

The simulation of a CO_2 tracer representing the emissions from the power plant alone is mandatory. Further CO_2 tracers representing the large-scale background or other anthropogenic emissions and biospheric fluxes in the domain are optional but recommended. High resolution models may include additional CO_2 tracers representing emissions from individual stacks (see section 3.2).

3. Input Data

3.1. Meteorology

The changing meteorological conditions during the simulation period should be captured as accurately as possible. Offline transport models (e.g. Lagrangian particle dispersion models) need to be driven by meteorological output from a numerical weather forecast model with hourly resolution. Ideally, the meteorological input data should be taken from a meteorological analysis/forecast (e.g. ECMWF operational data) at the highest possible spatial resolution (10 km or better). Higher spatial (<10 km) and temporal resolutions (< 1h) are recommended.

A set of input data (wind, temperature, pressure, humidity) at hourly and 1 km x 1 km resolution are provided from a reference COSMO-GHG simulation in netcdf format.

Online models producing their own meteorology should use ECMWF operational analyses as initial and boundary conditions as the default option. If nested into another regional simulation, the regional simulation itself should be nested into ECMWF analyses. Standard meteorological data assimilation/nudging within the domain of the online model should be turned on if possible.

3.2 Emissions

Emissions from Belchatow are released from two stacks, those from Jänschwalde from six of its nine cooling towers. All models need to include a CO_2 tracer representing the emissions from the power plant as a single source (denoted as "single" in Table 2). Models with resolutions better than 300 m should additionally include a tracer (or several tracers) released from the individual stacks to test the sensitivity of the results to this choice.

For Belchatow, the tracer "single" (see Table 2) should represent the sum of the emissions from the two stacks (East+West). For Jänschwalde, it should represent the sum of the emissions from only 3 instead of 6 locations (East+Centre+West), because the towers are arranged in 3 groups with 2 towers each. The distance between the groups is much larger (~300 m) than the distance between the 2 towers (~110 m) in each group.

The locations and the suggested CO_2 emission strengths of the sources are listed in Table 2. Note that the coordinates provided in E-PRTR are not the exact coordinates of the emissions but rather of the postal address of the plant. The source strengths correspond to the latest values reported to E-PRTR for the year 2017.

Table 2. Source locations and strengths (last 2 columns denote the same rate in different units)

Power plant	**Stack/tower**	**Coordinate** longitude, latitude	**Emission rate** [Mt CO_2/yr]	**Emission rate** [kg CO_2/s]
Belchatow	East	19.3285°E, 51.2660°N	19.2	608.8
Belchatow	West	19.3237°E, 51.2660°N	19.2	608.8
Belchatow	**Single**	19.3261°E, 51.2660°N	38.4 (2018)	1217.7
Jänschwalde	East	14.4622°E, 51.8360°N	7.7	244.2
Jänschwalde	Centre	14.4580°E, 51.8361°N	7.7	244.2
Jänschwalde	West	14.4538°E, 51.8362°N	7.7	244.2
Jänschwalde	**Single**	14.4580°E, 51.8361°N	23.1 (2018)	732.5

Emissions from the power plants undergo plume rise due to the momentum and buoyancy of the flue gas. Plume rise depends on stack and effluent parameters as well as on meteorological conditions (wind speed, stability).

Vertical emission profiles

Plume rise and the vertical extent of the plumes were calculated using the empirical equations recommended by the Association of German Engineers (VDI – Fachbereich Umweltmeteorologie, 1985), which are based on the original work of Briggs (1984). Typical stack parameters were obtained from Pregger et al. (2009), considering typical power plant capacities and fuel types, and from site descriptions (Table 3) .

Table 3. Stack parameters used in plume rise calculation.

Site	Stack height (m)	Stack diameter (m)	Effluent temperature (K)	Volume flux ($m^3 s^{-1}$)	Comment
JAE	120	NA	322	790	emission of filtered flue gas through cooling towers
BEL	299	NA	432	330	direct emissions through stack from combustion process

All models need to simulate three CO_2 tracers with fixed vertical emission profiles representing a high, middle and a low release case (tracers CO2_PP_H, CO2_PP_M and CO2_PP_L as described in section 2). The middle release case corresponds to the plume rise calculation for the approximate time of the aircraft measurement flights (07 Jun 2018 12:00 UTC for Belchatow, 23 May 2018 09:00 UTC for Jänschwalde), whereas the high case represents an upper limit of the plume rise calculation during the last 24 hour before the flights. The lower release height corresponds to the surface. In addition, an optional release at that height of the stack may be simulated as CO2_PP_S .

The vertical profiles are provided in the following files

plume_rise_BEL.csv

plume_rise_JAE.csv

The columns in the file are

tracer, E0_50, E50_100, E100_150, E150_200, ... , E1450_1500

where EXXX-YYY is the fractional emission from the altitude layer between XXX m and YYY m above ground. The sum over all layers is 1. Altitudes are meters above ground.

Models which simulate additional tracers for individual stacks should use the MID vertical profile for these tracers.

Models able to incorporate temporally changing emission profiles should additionally include a tracer CO2_PP_T representing the emissions from hourly changing profiles. Plume rise was computed for the full simulation periods from hourly profiles of wind and temperature from COSMO-GHG meteorological simulations at the locations of the two power plants.

Hourly emission profiles are provided in the following files

plume_rise_timeseries_BEL.csv

plume_rise_timeseries_JAE.csv

with columns

year, month, day, hour, min, E0_50,E50_100, E100_150, E150_200, … , E1450_1500

Models should update the profiles each hour (times in the files denote the start of the hour). If the simulation starts earlier than the first time available in the file (e.g earlier than 6 Jun 2018 00 UTC in case of Belchatow), then the first profile in the file should be used for all those early hours.

4. Output

To facilitate the processing and inter-comparison of the simulations, please follow the following guidelines for the file content and formats as closely as possible. Only gridded output is requested. Interpolation to the measurements is then done centrally in a unified way. Output should be generated on the native vertical grid of the model but horizontally interpolated to a regular latitude-longitude grid (using the WGS84 geodetic reference).

To account for the different resolutions and domain sizes, output should be provided for two different domains. The smaller inner domain fully encompasses the aircraft measurements and targets the near-field of the plumes. The larger outer domain extends about 100 km on all sides of the power plants.

Table 4. Output grids (all coordinates denote grid cell centers) and output frequency.

Power plant	**Domain**	**Longitude range**	**Latitude range**	**resolution** dlon x dlat	**Size** nx x ny	**Freq.** hr
Belchatow	SMALL	18.7– 19.9°E	50.95 – 51.55°N	0.003° x 0.002°	401 x 301	0.25[1]
Belchatow	LARGE	17.8 – 20.8°E	50.25 – 52.25°N	0.015° x 0.01°	201 x 201	1.00
Jänschw.	SMALL	13.8 – 15.0°E	51.50 – 52.10°N	0.003° x 0.002°	401 x 301	0.25[1]
Jänschw.	LARGE	12.9 – 15.9°E	50.80 – 52.80°N	0.015° x 0.01°	201 x 201	1.00

[1] *ARTM can only provide hourly output*

We ask you to provide output in netCDF format with **one file per day** containing the following dimensions and variables:

File name format: [ID]_[Domain]_[yyyymmdd]_[group]_[model].nc

Where ID is the simulation ID (e.g. BEL_M), domain is either SMALL or LARGE. Group can be e.g. DLR, model e.g. EULAG. Please use capital letters. In case of multiple simulations, please include the simulation version in the model name, e.g. EULAG-SIM1.

Dimensions:

- latitude: number of latitudes
- longitude: number of longitudes
- level: vertical level number
- time: number of time steps

Coordinate variables:

- Latitude: degrees north

longitude: degrees east

time: days since 01 Jan 2018 00:00 (UTC)

2D variables (single precision):

ZSURF: Surface altitude (m)

PS: Surface pressure (Pa)

3D variables (single precision):

Z: altitude above sea level / geopotential height (m)

p: pressure (Pa)

T: temperature (K)

Q: specific humidity (kg/kg)

U: east-west wind component (m/s)

V: north-south wind component (m/s)

CO2_XYZ: CO2 dry air mole fraction (mol/mol)

Variables constant in time can be provided without time dimension, but need to be included in each daily file. All other variablesXLA need to include the dimension *time*.

For hourly output, a daily file should contain output for 0 UTC, 1 UTC, … , 23 UTC, where the time corresponds to the instantaneous model fields (or center of an averaging interval). Output at 15 minute resolution should be provided in an analogous way for 00 UTC, 00:15 UTC, 00:30 UTC etc.

The vertical model domain should at least cover altitudes up to 2400 m above sea level.