

An online emission module for atmospheric chemistry transport models: Implementation in COSMO-GHG v5.6a and COSMO-ART v5.1-3.1

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Response to the Reviewer's Comments

We thank the two reviewers for their critical assessment and useful comments to improve the quality of our paper. In the following we address their concerns point by point. Changes in the paper are shown in blue.

Reviewer 1

5 **Reviewer Point P 1.1** — Figure 1 and section 2:

Please indicate the file format of the data listed in the parallelograms.

If I understood it correctly, the python tool is responsible for generating the emission and temporal and vertical profiles NetCDF files that are later read by the online emission module. Nevertheless, in Figure 1 it is not clear which information/files are used to generate this NetCDF files (e.g. in which format are the emission and temporal/vertical profiles originally provided by the user to the Python tool). Similarly, the description and process for generating these NetCDF files (e.g. `gridded_emissions_nc`, `hour_of_day_nc`, `day_of_week_nc`, ...) should be included in section 2 and corresponding subsections (right now the description of the files is included in section 3.1).

Reply: Figure 1 has been revised following the reviewer's suggestions. The file format of each dataset (grey parallelograms) is now indicated. The input files for temporal and vertical profiles as well as speciation factors (for COSMO-ART) now also appear in the first input data box. Data produced by the Python tool or int2lm are labeled with "output". Furthermore, the overall formatting of the figure has been improved for better readability.

The description of the netCDF files generated by our Python tool has been moved to Section 2:

The generated netCDF files contain time functions of diurnal, day-of-week and seasonal variations per tracer and source category. These scalings are provided in three separate files by default. However, it is also possible to provide only one file with hour-of-year scaling factors. The temporal profile variables are arrays with the two dimensions `time` (e.g. 24 different `hourofday` in case of a diurnal profile) and `country`. If no country-specific information is available or desired, a uniform country mask with a single

value for the whole model domain needs to be generated. Vertical profiles, in contrast, are 1D arrays with `level` as the only dimension, since they are not expected to vary with country.

Further:

The file generated by the Python tool contains vertical profiles per tracer and source category. The number of levels and their heights above surface can be set independently of the vertical structure of the COSMO grid.

In Section 3, a table has been added to link the variable names within these files with the namelist tags:

Table 1. Overview of netCDF files and corresponding namelist tags in the `TRACER` group in `INPUT_GHG` or `INPUT_OAE`. The netCDF variable names must be identical to those listed in the namelist members (right column).

Variable for netCDF file name	Namelist member
<code>gridded_emissions_nc</code>	<code>ycat1</code>
<code>hour_of_day_nc</code>	<code>ytpl</code>
<code>day_of_week_nc</code>	<code>ytpl</code>
<code>month_of_year_nc</code>	<code>ytpl</code>
<code>hour_of_year_nc</code>	<code>ytpl</code>
<code>vertical_profile_nc</code>	<code>yvpl</code>

Reviewer Point P 1.2 — Section 2.1 – gridded emission inventories:

Perhaps this section should be accompanied with a table that list the different inventories that are currently available for processing and their main characteristics (e.g. name of inventory, pollutants considered, sector classification, year(s) of reference, spatial resolution-coverage, reference).

In its current version, the presented tool is capable of processing three different families of anthropogenic inventories (TNO, EDGAR and Swiss national inventory). I understand that other types of emissions such as biogenic or ocean are estimated/incorporated into COSMO using other specific models/tools (e.g. MEGAN for BVOCs), but what about biomass burning emissions (e.g GFAS or GFED)? Are they being estimated using an online approach inside COSMO?

Reply: From our point of view, an overview table of the different inventories would not be helpful, since we would like to emphasize the flexible and generic nature of our implementation rather than presenting a tool that is tailored to specific types of inventories. The inventories currently supported are explained and referenced in the text. Furthermore, emission

inventories change quite rapidly: new versions are released, formats change, additional years and species are covered, etc. The modularity and flexibility of our tool allows such changes to be incorporated rather quickly.

Certain types of natural emissions are indeed implemented in specific modules in COSMO-ART, but emissions from natural fires are not. They have been accounted for in previous simulations using the traditional offline approach. Since biomass burning emissions do not follow a regular spatio-temporal pattern, our online emissions processing tool is not suitable for this type of emissions. We are aware that this is an important shortcoming. An extension of the tool to support a combination of offline inputs and online computation would be straightforward (since both methods are already implemented as separate options), but this is currently not implemented. We added the following sentence in the conclusions section:

Our tool is tailored to the processing of anthropogenic emissions, which follow a regular pattern in space and time, but it is not suitable for the processing of highly variable emissions such as emissions from biomass burning. This will require an extension to support a combination of offline inputs and online computation.

Reviewer Point P 1.3 — Section 2.2 and 2.3:

Temporal, vertical and speciation profiles are being applied to gridded emissions. Therefore, all the equations of these sections should represent emission of a tracer X at time t and grid cell c (instead of only tracer X at time t).

Reply: In Section 2.3 (former Section 2.2) we state that "This formula is applicable to an emission from a single grid cell or to a complete 2D emission field; [...]" and thus, the additional index is not necessary here.

Reviewer Point P 1.4 — Section 2.4:

Why the grid cell areas are calculated in degree? There are tools like CDO (Cdoorbpy for Python) that allow calculating grid cell areas in m². It is currently not clear with which tools/libraries is the emission conservative mapping being performed (e.g using ESMF? Specific python libraries that allow creating geometric objects, such as shapefiles, and subsequently performing spatial interpolations?)

Following with the previous sections (2.2 and 2.3), an equation illustrating how the emissions are being mapped from the source grid cells onto destination grid cells should be included.

Reply: To map emissions from the inventory to the model grid, we use our own implementation that makes use of the shapely and cartopy library. For each cell from the inventory and the COSMO grid, we produce a shapely polygon and use the "intersection" method to compute the intersection between the two. The intersection has an "area" method returning the area of the intersection. Grid cell areas were only calculated in degrees for computing the overlap between a COSMO grid cell and an inventory grid cell. However, we modified the implementation to first project the polygons into the Mollweide equal-area projection, solving this issue. This has virtually not changed the results (maximum ratio difference of $3 \cdot 10^{-5}$).

We have moved this Section to 2.2 and revised it to clarify these points:

All emission data need to be mapped onto the simulation grid, which in case of COSMO is a rotated latitude-longitude grid. Such mapping is straightforward for point sources for which the emissions are added to the COSMO grid cells that contain the sources. For area sources this is less trivial, since simple interpolation is not mass-conservative, whereas conservative nearest neighbor methods may lead to undesired stripes or other discontinuities. In order to avoid such issues and to accurately conserve mass, we determine for each COSMO grid cell the relative fraction of the overlap with each inventory grid cell. The emissions for all source categories s at each COSMO grid cell i are then computed by

$$E_{i,s}^{\text{COSMO}} = \sum_{j=1}^N f_{i,j} \cdot E_{j,s}^{\text{inventory}} \quad (1)$$

where $E_{i,s}^{\text{COSMO}}$ and $E_{j,s}^{\text{inventory}}$ are the emissions (in mass/cell) at the i -th and j -th COSMO and inventory grid cell, respectively, N is the number of grid cells in the inventory and $f_{i,j}$ is the dimensionless fraction of the source cell j contributing to destination cell i . The fraction is determined by computing the intersection between each COSMO and inventory grid cell divided by the total area of the inventory cell using the equal-area Mollweide projection to conserve the mass.

Our tool does not redistribute the low-resolution inventory data onto the high-resolution COSMO-grid using additional information, such as land-sea masks and country boundaries, which can be used for improving the spatial allocation of area sources. This feature could be implemented in a future version similar to the implementation in CHIMERE-2017 model (Mailler et al., 2017).

The generated netCDF file contains 2D gridded fields $E_{i,s}$ directly on the COSMO grid. This file also contains a corresponding 2D country mask, which is an integer field with each grid cell being assigned the number of the country that has the largest fractional area. The unit of the emissions $E_{i,s}^{\text{COSMO}}$ depends on the actual model and are converted accordingly. For example, COSMO-GHG expects $\text{kg m}^{-2} \text{s}^{-1}$, whereas emissions in COSMO-ART are in $\text{kg h}^{-1} \text{cell}^{-1}$.

Reviewer Point P 1.5 — Section 3.3.1:

How are separated the emissions when there are several countries into a cell (i.e. country border cells)? Or it is assumed that all emissions belong to the country that contains the largest fraction of the cell? Some inventories like TNO provide the information of emissions per grid cell and emitting country. Is this information used when given?

Reply: When running the COSMO online emission module, the assumption is made that the country mask attributes a single country to each grid cell. This country is indeed the one containing the largest fraction of the cell. However, this only impacts the temporal profile applied to the cell, which can be country dependent.

In regard to the emissions, if a grid cell from the TNO inventory covers multiple countries, there are indeed multiple entries in the inventory. Those are summed and the regridding is applied to the sum. Therefore, emissions from one country

can be partially assigned to the neighbouring country and vice versa. This is also the case for cells bordering the sea, as noted in the Reviewer Point P 2.1. Note that point source emissions are still attributed to the correct COSMO grid cell. A mention of this limitation has been added to the Section 2.2:

Our tool does not redistribute the low-resolution inventory data onto the high-resolution COSMO-grid using additional information, such as land-sea masks and country boundaries, which can be used for improving the spatial allocation of area sources. This feature could be implemented in a future version similar to the implementation in CHIMERE-2017 model (Mailler et al., 2017).

Reviewer Point P 1.6 — Conclusion and Table 4 results:

According to the results presented in Table 4, the main advantage of using the online emission module instead of the offline tool is the significant reduction of the disk storage. Both in the COSMO-ART and COSMO-GHG test cases, authors suggest that increasing the length of the simulation period would imply a proportional growth of the benefit in disk usage. This very much would depend on how the workflow of the modelling system is set up. For instance, when running a 1-year simulation with an offline emission tool, modelers tend to generate an emission file of 24 hours for day “d”, then run the atmospheric chemistry model for day “d”, erase the emission file for day “d”, generate an emission file of 24 hours for day “d+1”, run the atmospheric chemistry model for day “d+1” and so on. In this situation, the benefit in disk usage would remain the same regardless of the simulation period (i.e. you will always be storing only one emission file of 24 hours). Having said that, I think the authors should include the time required for data pre-processing when comparing the off-line and online approach. Otherwise the comparison remains unfair: the online computation of hourly emissions is considered but the offline computation of hourly emissions is not, which is also part of the modelling chain. Finally, the values reported for the simulation times should be split between time required to compute hourly emissions (online/offline), time spent on I/O and “others”. This would allow to justify the suggested compensation between I/O decrease and computation increase reported by the authors.

Reply: Thank you for this important comment. We agree that storage size can be controlled by a more sophisticated workflow as you described. However, the amount of data that needs to be read in remains the same. This is why we refer to it as "input size" in Table 4 in particular. Reduced data storage is by far not the only advantage. From our view, the largest advantage is the greatly simplified workflow, since we don't need to produce new input files for every new simulation (unless we change domain size etc.). This is also what we state first when summarizing the advantages of the tool in the Conclusions.

To further specify the processing times required for pre-processing, we added another table showing the difference in all relevant pre-processing steps for online and offline processing, respectively. Unfortunately, the simulation times cannot be split since this information is not available.

Table 2. Benchmark for pre-processing online and offline emissions for the COSMO-GHG test case using the emiproc tool. Altogether, 19 categories from the emission inventories were processed (TNO: 14, Swiss: 5) as input for the CO₂ tracer. Pre-processing was performed on a local Linux cluster, using 14 threads in parallel. Processing times for generating the mapping and country mask file are excluded. Results are shown for different time periods.

Processing step	Processing time (s)		
	1 day	7 days	365 days
Mapping and merging of inventories, profile generation	78	78	78
Offline Processing: extracting data from profiles (netCDF)	106	106	106
Offline Processing: generating offline files	11	74	3859
Total Online	78	78	78
Total Offline	117	180	3965
Ratio Online / Offline	0.67	0.43	0.02

Reviewer Point P 1.7 — Meteorological parametrizations:

Besides the improvement shown by the authors in terms of disk storage, one would say that the main advantage of building an online emission module is the capability of computing on-line meteorological parametrizations such as heating degree day (for temporally distributing residential heating emissions) or plume rise calculation (for vertically distributing point source emissions). Scientifically (and even technically) speaking, the gains of performing such an implementation in comparison to an off-line approach may be much more significant. I understand that such an implementation may be more complex/time consuming than the one presented in this work, but perhaps it would be good to highlight it as a current limitation of the current tool and the need to work on it in the near future.

Reply: As pointed out in our reply to Reviewer Point P 1.6, the largest advantage of the tool is actually not the reduced storage demand but the simplified workflow. But we agree with the reviewer that a particularly attractive advantage of an online processing tool is the possibility to link the emissions to the actual meteorology in the model. This has indeed not yet been implemented and should be a focus of future developments. We added the following sentence at the end of the Conclusions section:

Future developments will focus on the porting to other model systems such as ICON-ART and on the implementation of meteorology-dependent emissions such as emissions from residential heating or from lightning.

Reviewer Point P 1.8 — Portability to other atmospheric transport models:

Authors suggest that the offline python package is of potential use for any atmospheric transport model system. I think this statement may be too strong in its current formulation, especially considering that each model requires the

emissions to be provided following specific file formats (e.g. specific attributes in the NetCDF files) and conventions (e.g. units), and that certain models (e.g. WRF-CHEM, CMAQ) work with map projections that are currently not supported by the python package (e.g. lambert conformal conic, Mercator). Moreover, the current offline approach includes a COSMO pre-processor tool to perform a vertical interpolation to the model levels. How this vertical
5 interpolation would be performed in other models?

Reply: We are convinced that adaptations to other model systems require only a small effort. If users want to generate emissions for different inventories and/or different transport models, they can implement their own classes within emiproc in a straightforward manner by modifying the existing examples. Also, any map projection available in the cartopy package can easily be utilized (including Lambert Conformal conic and Mercator). Units and attributes of the output netCDF variables
10 are already model-dependent. For example, COSMO-GHG expects emissions in $\text{kg m}^{-2} \text{s}^{-1}$, whereas in COSMO-ART it is $\text{kg h}^{-1} \text{cell}^{-1}$, which is implemented in emiproc.

Note that the pre-processing does not interpolate the emissions to the vertical levels of the COSMO-model but to any pre-defined set of vertical levels. Interpolation to the terrain-following 3D grid of the COSMO-model is accomplished online as explained in Section 3.2. The same approach will have to be followed for any other model with terrain-following
15 vertical coordinates.

Based on the reviewer's suggestion, we adjusted the text in the introduction referring to the offline tool as follows:

Models and inventories that are currently not covered by the Python package can be implemented in a straightforward manner.

Reviewer Point P 1.9 — Supplementary material:

20 Table S-1 to S-5: please specify from which works/references are the profiles derived.

COSMO-GHG example namelist includes some namelist members that are not defined in Table 3 of the manuscript or in the text (e.g. `itype_1bc`). Please provide a description of them (or remove them if they are not relevant to the publication).

In order to illustrate how "contribl" is used for chemical speciation, can you also provide a COSMO-ART example
25 namelist?

Reply: The following sentences have been added to the supplement:

Vertical profiles are based on source-specific profiles developed for the European Monitoring and Evaluation Program (EMEP) (Bieser et al., 2011) that have been modified for the SMARTCARB project (Brunner et al., 2019).

30 and

The time profiles of emissions were originally published by TNO for SNAP emission categories (Denier van der Gon et al., 2011; Pouliot et al., 2012) and have been mapped to GNFR categories within the CHE project (Haussaire et al., 2018).

Originally, we wanted to provide a complete namelist example. However, as pointed out by the reviewer, some namelist members are not relevant for this publication. Thus, they have been removed from the example. Furthermore, we added a COSMO-ART example namelist for speciation of NO_x into NO₂ to show the usage of `contrib1`.

Minor

Reviewer Point P 1.10 — Please specify the units of `Ex(t)`, `Ex,s` and `fx,s`

Reply: Units for emissions, scaling and speciation factors have been added.

10 **Reviewer Point P 1.11** — Table 3: Why `itype_emiss` and `itype_tscale` are only needed for COSMO-GHG?

Reply: In COSMO-ART, the use of online (or offline) emissions cannot be specified for each tracer separately. Instead, there is a general Boolean switch `itype_emiss` to activate online emission processing for all tracers. COSMO-ART only supports method 1 of the namelist flag `itype_tscale`, i.e. "temporal scaling using hour of day, day of week and month of year". Therefore, the flag `itype_tscale` cannot be set. We added the following text in Section 3.1 to clarify these points:

For this reason, the namelist switch `itype_emiss` does not exist in COSMO-ART. The same applies for `itype_tscale`, since temporal scaling is applied just for hour-of-day, day-of-week and month-of-year profiles.

20 **Reviewer Point P 1.12** — Figure 2 caption, please include the meaning of each polygon shape/colour (following the example of Figure 1's caption).

Reply: Done.

25 **Reviewer Point P 1.13** — Please, add the following reference to the CAMS-REG-APV2_2 inventory: Granier, C., Darras, S., Denier van der Gon, H.A.C., Doubalova, J., Elguindi, N., Galle, B., Gauss, M., Guevara, M., Jalkanen, J.-P., Kuenen, J., Lioussé, C., Quack, B., Simpson, D., and Sindelarova, K.: The Copernicus Atmosphere Monitoring Service global and regional emissions (April 2019 version), Copernicus Atmosphere Monitoring Service (CAMS) report, 2019, doi:10.24380/d0bn-kx16, 2019

Reply: Thank you for this suggestion. We added this reference.

Reviewer Point P 1.14 — In the introduction, when listing currently available emission processing systems, I would suggest to also mention the HEMCO system: Keller, C. A., Long, M. S., Yantosca, R. M., Da Silva, A. M., Pawson, S., and Jacob, D. J.: HEMCO v1.0: a versatile, ESMF-compliant component for calculating emissions in atmospheric models, *Geosci. Model Dev.*, 7, 1409–1417, <https://doi.org/10.5194/gmd-7-1409-2014>, 2014

5 **Reply:** This is indeed an important reference that was missing. We added the reference as suggested.

Reviewer 2

Reviewer Point P 2.1 — The authors do not explain how they take into account the distinction between land and sea. No discussion is provided on that point. Lines 11-12, p. 6 suggest that the emission for any, possibly coarse, cell of the input inventory will be assumed to be evenly distributed within this cell, and thereafter evenly
10 redistributed between all the intersecting model cells according to the intersection area. In the common case when model cell is smaller than inventory cell, this would lead to emissions of a clearly continental nature (e.g. traffic, residential heating) ending up in part in purely oceanic model cells, and shipping emissions ending up in part in purely continental cells. The authors should either explain how they avoid this problem, or acknowledge this point as a serious limitation of their tool that needs to be addressed in its future versions.

15 **Reply:** Thank you for this important comment. Our current version does not use additional information (land/sea mask, landuse etc.) to redistribute low-resolution inventory data onto the high-resolution COSMO-grid. We have modified the section and now mention this limitation:

Our tool does not redistribute the low-resolution inventory data onto the high-resolution COSMO-grid using additional information, such as land-sea masks and country boundaries, which can be used for
20 improving the spatial allocation of area sources. This feature could be implemented in a future version similar to the implementation in CHIMERE-2017 model (Mailler et al., 2017).

Reviewer Point P 2.2 — Similar to point 1 (but less hindering), accounting for landuse differences to have a meaningful distribution of emissions among model cells is also possible (e.g. the emiSURF emission preprocessing tool described in Mailler et al., 2017, "CHIMERE-2017 : from urban to hemispheric chemistry-transport modeling").
25 From a computational point of view this would be the same as accounting for land/ocean difference, but less critical. If the inventory is, e.g., 10x10km, one inventory cell could very well contain one area with forest and one city, and taking this information into account when generating emissions at the, say, 1x1km resolution of the model is clearly

useful. Same as for point 1., if this is done the authors should explain how, and if not they should acknowledge this point as a limitation compared to other tools.

Reply: See our previous response.

- Reviewer Point P 2.3** — I can take the word of the authors that it does not generate major errors, but the areas in square degrees are not really convincing. An "area" in squared degrees is not an area, and is not even proportional to the geometric area (that would depend on the orientation of the considered area, zonally or meridionally elongated). It would probably not be more difficult to work with real geometric areas on a sphere. The meaning of an area in squared degrees is really unclear to me, in particular if either the inventory or the model grid is not a regular lat-lon grid. What is a square degree close to the pole for example ? I feel uncomfortable with this point which more or less prevents a clear and physical writing of the equations for horizontal redistribution of the emissions, which are the key points of the tool they propose. In my opinion, the code should be slightly modified to deal with real geometric areas in squared meters.

Reply: We addressed this issue already in our reply to Reviewer Point P 1.4. We have modified the code to compute the intersection in an equal-area projection, solving this issue.

- Reviewer Point P 2.4** — The country-dependance of time profiles is mentioned in the text but not in the equations. As a consequence, the management of cells that are at the border of two or more countries is not really made clear : does the CTM have, for these cells, yearly amount of pollutant per snap sector *and per country* ? This problem is not major, but the authors should make clear how they deal with this issue

Reply: We addressed this issue already in our reply to Reviewer Point P 1.5.

References

- Bieser, J., Aulinger, A., Matthias, V., Quante, M., and van Der Gon, H. D.: Vertical emission profiles for Europe based on plume rise calculations, *Environmental Pollution*, 159, 2935–2946, <https://doi.org/10.1016/j.envpol.2011.04.030>, <http://www.sciencedirect.com/science/article/pii/S0269749111002387>, 2011.
- 5 Brunner, D., Kuhlmann, G., Marshall, J., Clément, V., Fuhrer, O., Broquet, G., Löscher, A., and Meijer, Y.: Accounting for the vertical distribution of emissions in atmospheric CO₂ simulations, *Atmospheric Chemistry and Physics*, 19, 4541–4559, <https://doi.org/10.5194/acp-19-4541-2019>, <https://www.atmos-chem-phys.net/19/4541/2019/>, 2019.
- Denier van der Gon, H., Hendriks, C., Kuenen, J., Segers, A., and Visschedijk, A.: Description of current temporal emission patterns and sensitivity of predicted AQ for temporal emission patterns: TNO Report, EU FP7 MACC deliverable report
- 10 D_D-EMIS_1.3, Report, MEP-R2003/166, Apeldoorn, The Netherlands, 2011.
- Haussaire, J.-M., Brunner, D., Marshall, J., Prunet, P., Augusti-Panareda, A., Manders, A., Segers, A., Denier van der Gon, H., Maenhout, G., Houweling, S., and Krol, M.: CHE Deliverable 2.1 - Model systems and simulation configurations, Version 2.0, Tech. rep., CO₂ Human Emissions Project, <https://www.che-project.eu/sites/default/files/2018-04/CHE-D2-1-V2-0.pdf>, 2018.
- 15 Mailler, S., Menut, L., Khvorostyanov, D., Valari, M., Couvidat, F., Siour, G., Turquety, S., Briant, R., Tuccella, P., Bessagnet, B., Colette, A., Létinois, L., Markakis, K., and Meleux, F.: CHIMERE-2017: from urban to hemispheric chemistry-transport modeling, *Geoscientific Model Development*, 10, 2397–2423, <https://doi.org/10.5194/gmd-10-2397-2017>, <https://www.geosci-model-dev.net/10/2397/2017/>, 2017.
- Pouliot, G., Pierce, T., van der Gon, H. D., Schaap, M., Moran, M., and Nopmongcol, U.: Comparing emission inventories and
- 20 model-ready emission datasets between Europe and North America for the AQMEII project, *Atmospheric Environment*, 53, 4 – 14, <https://doi.org/https://doi.org/10.1016/j.atmosenv.2011.12.041>, <http://www.sciencedirect.com/science/article/pii/S1352231011013288>, 2012.

An online emission module for atmospheric chemistry transport models: Implementation in COSMO-GHG v5.6a and COSMO-ART v5.1-3.1

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Abstract. Emission inventories serve as crucial input for atmospheric chemistry transport models. To make them usable for a model simulation, they have to be pre-processed and, traditionally, provided as input files at discrete model time steps. In this paper, we present an “online” approach, which produces a minimal number of input data read in at the beginning of a simulation and which handles essential processing steps online during the simulation. For this purpose, a stand-alone Python package “emiproc” was developed, which projects the inventory data to the model grid and generates temporal and vertical scaling profiles for individual emission categories. The package is also able to produce “offline” emission files if desired. Furthermore, we outline the concept of the online emission module (written in Fortran 90) and demonstrate its implementation in two different atmospheric transport models, COSMO-GHG and COSMO-ART. Simulation results from both modeling systems show the equivalence of the online and offline procedure. While the model run-time is very similar for both approaches, ~~disk~~ storage-input size and pre-processing time are greatly reduced when online emissions are utilized.

1 Introduction

Gridded and temporally varying emission fields are a critical input for three-dimensional atmospheric chemistry transport models (Matthias et al., 2018). Traditionally, such emissions are obtained from an inventory and pre-processed for the model as external inputs, which are read in during simulation at regular time steps. The pre-processing typically includes a mapping of the inventory to the model grid and the application of temporal and vertical profiles depending on emission source category. In case of atmospheric chemistry models, a speciation, i.e. a mapping of the species in the inventory to those simulated in the model is required, for example the mapping of total non-methane volatile organic compounds (NMVOCs) to individual NMVOC species. A prominent example of an emission pre-processing model is the Sparse Matrix Operator Kernel Emissions model (SMOKE, <https://www.cmascenter.org/smoke/>), which has been used extensively with different atmospheric chemistry models in the United States (McHenry et al., 2004; Wong et al., 2012), Europe (Borge et al., 2008; Bieser et al., 2011a), and Asia (Wang et al., 2011). More recent examples are the pre-processor PREP-CHEM-SRC (Freitas et al., 2011) ~~and~~ the

High-Effective Resolution Modelling Emission System ~~HERMES-Guevara et al. (2019)~~[\(HERMES; Guevara et al., 2019\)](#) and [the Harvard-NASA Emission Component v1.0 \(HEMCO; Keller et al., 2014\)](#).

In case of a large number of tracers and hourly input, the pre-processing and reading of the emission fields (hereafter referred to as “offline approach”) imposes a large computational burden in terms of input and output (I/O) operations and storage. An alternative is to apply the temporal and vertical profiles inside the model (“online approach”), which greatly reduces the number and size of input files and the corresponding I/O. This approach enhances the flexibility in setting up new model simulations since no new emission data need to be generated before the start of a simulation. Furthermore, meteorology-dependent emissions, such as emissions from residential heating depending on outdoor temperatures, can be incorporated more easily.

Here we present such an online emission module, which has been integrated into two different atmospheric transport models, both based on the regional numerical weather prediction and climate model COSMO (Consortium for Small-scale Modeling; Baldauf et al., 2011). The first model was developed for the passive transport of tracers such as long-lived greenhouse gases, and is referred to as COSMO-GHG (Liu et al., 2017; Brunner et al., 2019). The second model is COSMO-ART (Aerosols and Reactive Trace gases; Vogel et al., 2009; Knöte et al., 2011), which simulates the transport and chemistry of reactive gases and aerosols as well as two-way feedbacks between meteorology and chemistry. Both are fully integrated, online coupled models simulating the meteorology and the transport (and chemistry) of atmospheric constituents consistently in one single model (Baklanov et al., 2014). The module has also been incorporated into the model COSMO-ART-M7 (Glassmeier et al., 2017), which extends COSMO-ART with an optional simplified chemistry and aerosol scheme for climate applications, but this implementation will not be discussed here.

The purpose of this study is to present the conceptual framework of the online emission module, to demonstrate its suitability and flexibility for the simulation of greenhouse gases and air pollutants, and to show its equivalence to the traditional offline approach. Although the implementation of the module is specific to COSMO, the overall concept is generic and the code has been written in a modular way to facilitate integration into other (Fortran-based) model systems, for example as an extension to the recently developed emission module for ICON-ART (Weimer et al., 2017). The online module is composed of one Fortran module file, which interfaces with several routines of the standard COSMO model and its extensions GHG and ART as described later.

Furthermore, a separate Python package generates a small number of input files required for the simulation. Different from the offline approach, these files are read in only once at the beginning of a simulation. The Python package also supports the generation of hourly input files for offline applications. This capability is used here to compare simulations with online and offline emission processing. In contrast to the Fortran module, the Python package is independent of the specific model implementation and, therefore, of potential use for ~~any other~~ atmospheric transport model system. [Models and inventories that are currently not covered by the Python package can be implemented in a straightforward manner.](#)

The manuscript is organized as follows: Section 2 describes the functionality of the Python pre-processing package. Section 3 presents the implementation of the online emission module in the modeling systems COSMO-GHG and COSMO-ART and

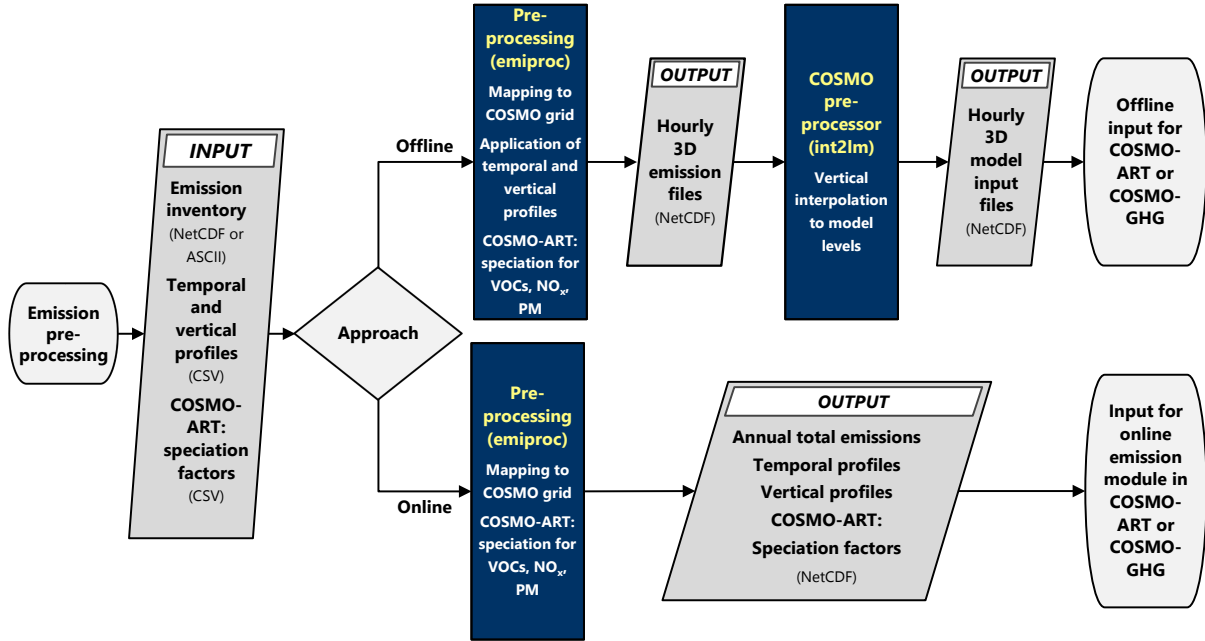


Figure 1. Flow chart of the emission pre-processing for both offline and online approaches as implemented in COSMO-GHG/ART. Dark grey parallelograms represent data (with input or output indicated). Blue rectangles are processing scripts. Start and end points are represented by ovals.

demonstrates its advantages based on three practical examples. Finally, [Section Sect. 4](#) shows a performance assessment for both offline and online processing and demonstrates the equivalence of the two approaches based on two example simulations.

2 Emission pre-processing

For the pre-processing of the input data required by COSMO, a separate Python-based tool named “emiproc” has been developed. The tool provides the mapping of gridded emission inventories to any desired COSMO grid (latitude-longitude grid with a rotated pole) or regular latitude-longitude grid. Other projections could be implemented easily. It also generates the temporal and vertical profiles needed for the online computation of emissions. If desired, the tool is able to generate offline emissions, which may be useful for users if no online emission module is implemented in their model.

The overall workflow of the emission pre-processing is illustrated in Fig. 1 for both approaches. In case of offline emissions, an additional step is required for the interpolation to the vertical grid of COSMO, which is executed by the official COSMO pre-processing tool int2lm (http://www.cosmo-model.org/content/model/documentation/core/int2lm_2.05.pdf). Int2lm also merges the emission fields with other COSMO inputs such as initial and boundary conditions and ensures proper formatting of the files.

2.1 Gridded emission inventories

Emission inventories of greenhouse gases and air pollutants are usually provided as annual 2D gridded fields per source category (e.g., traffic, industry, residential, agriculture) (Kuenen et al., 2014; Janssens-Maenhout et al., 2017; Crippa et al., 2018). Before incorporating these emissions into a 3D atmospheric transport model, the 2D fields have to be convolved with temporal profiles of diurnal, day-of-week, and seasonal variability as well as with vertical emission profiles (Denier van der Gon et al., 2011; Pouliot et al., 2012; Kuenen et al., 2014). Current approaches for the definition of temporal and vertical profiles are often highly simplified (Matthias et al., 2018), partly due to a lack of detailed information but also due to the limited flexibility offered by the offline approach.

Our current implementation of the module supports three different families of emission inventories: the inventories of the Netherlands Organization for ~~applied scientific research TNO~~ [Applied Scientific Research \(TNO\)](https://www.tno.nl/en/our-work/energy-environment/air-quality), the EDGAR inventories of the European Joint Research Centre (JRC), and the Swiss national emission inventories generated by Meteotest Inc., Switzerland. An extension to similar gridded inventories should be straightforward.

Although the inventories share a similar logic, there are distinct differences that had to be accounted for: In Europe, the two most prominent source classifications are the Standardized Nomenclature for Air Pollutants (SNAP; Centre on Emission Inventories and Projections (CEIP), 2018) and gridded Nomenclature for Reporting (GNFR; United Nations Economic Commission for Europe, 2015; Schindlbacher et al., 2016). SNAP is an old standard introduced in the context of the Convention on Long-Range Transboundary Air Pollution (CLRTAP), which had been used for many years in inventories produced by the European Monitoring and Evaluation Programme (EMEP) and by TNO. The latest inventories, however, follow the EMEP/CORINAIR NFR, which was introduced to harmonize the source classification with the one used in National Inventory Reports to the United Nations Framework Convention for Climate Change (UNFCCC EEA, 2000). For gridded inventories, the large number of NFR categories are usually lumped into 13 individual classes (A–M). This reduced set of categories is commonly referred to as gridded NFR or GNFR. EDGAR inventories are reported as individual or lumped NFR categories, which are similar but not identical to the GNFR standard. A table for unambiguous mapping between individual NFR, GNFR and SNAP categories is available at United Nations Economic Commission for Europe (2003).

Another difference is the map projection. EDGAR and TNO inventories are reported on a regular latitude-longitude grid, the Swiss Meteotest inventories on a Cartesian grid in the Swiss CH1903 Oblique Mercator projection. Furthermore, TNO inventories differentiate between point and area sources, which is not done in the other inventories. Point sources as reported to the European Pollutant Release and Transfer Register E-PRTR (<https://prtr.eea.europa.eu>) are provided in the TNO inventories at their exact location, which has the advantage that in high resolution simulations the point sources can be assigned accurately to the respective model grid cell. In addition, this allows applying separate vertical profiles to point and area sources as shown in Sect. 3.3.2.

2.2 [Mapping to COSMO grid](#)

All emission data need to be mapped onto the simulation grid, which in case of COSMO is a rotated latitude-longitude grid. Such mapping is straightforward for point sources for which the emissions are added to the COSMO grid cells that contain the sources. For area sources this is less trivial, since simple interpolation is not mass-conservative, whereas conservative nearest neighbor methods may lead to undesired stripes or other discontinuities. In order to avoid such issues and to accurately

5 conserve mass, we determine for each COSMO grid cell the relative fraction of the overlap with each inventory grid cell. The emissions for all source categories s at each COSMO grid cell i are then computed by

$$E_{i,s}^{\text{COSMO}} = \sum_{j=1}^N f_{i,j} \cdot E_{j,s}^{\text{inventory}} \quad (1)$$

where $E_{i,s}^{\text{COSMO}}$ and $E_{j,s}^{\text{inventory}}$ are the emissions (in mass/cell) at the i -th and j -th COSMO and inventory grid cell, respectively. N is the number of grid cells in the inventory and $f_{i,j}$ is the dimensionless fraction of the source cell j contributing to destination cell i . The fraction is determined by computing the area of the intersection between each COSMO and inventory grid cell divided by the total area of the inventory cell using the equal-area Mollweide projection to conserve mass.

10

Our tool does not redistribute the low-resolution inventory data onto the high-resolution COSMO grid using additional information, such as land-sea masks and country boundaries, which can be used for improving the spatial allocation of area sources. This feature could be implemented in a future version similar to the implementation in CHIMERE-2017 model

15 (Mailler et al., 2017).

The generated netCDF file contains 2D gridded fields $E_{j,s}$ directly on the COSMO grid. This file also contains a corresponding 2D country mask, which is an integer field with each grid cell being assigned the number of the country that has the largest fractional area. The unit of the emissions $E_{i,s}^{\text{COSMO}}$ depends on the actual model and is converted accordingly. For example, COSMO-GHG expects $\text{kg m}^{-2} \text{s}^{-1}$, whereas emissions in COSMO-ART are in $\text{kg h}^{-1} \text{cell}^{-1}$.

20 2.3 Temporal and vertical profiles

The emission of a tracer X at time t is calculated as the sum over the emissions per source category scaled with source-specific temporal scaling factors. A tracer is defined here as a quantity that is transported in the model, which can be a single trace gas or aerosol component, a composition of several species, or an idealized tracer. The temporal scaling factor for tracer X , source category s and time t is generally given by

$$25 \quad w_{X,s}(t) = w_{X,s,h}(h(t)) \cdot w_{X,s,d}(d(t)) \cdot w_{X,s,m}(m(t)) \quad (2)$$

where $w_{X,s,h}$, $w_{X,s,d}$ and $w_{X,s,m}$ are diurnal, day-of-week and seasonal scaling factors, respectively. The three scaling functions are dimensionless and have a mean value of 1, such that the mean value of all scaling factors applied to a full year of data is one (or very close to one). The step functions $h(t)$, $d(t)$, and $m(t)$ are the hour of the day, the day of the week, and the month of the year corresponding to the continuous time t , respectively. The emission of X at time t is thus

$$30 \quad E_X(t) = \sum_{s=0}^n E_{X,s} \cdot w_{X,s}(t) \quad (3)$$

where $E_{X,s}$ is the annual mean emission flux of X of source category s (which is the basic field usually provided by an inventory), and n is the total number of source categories. This formula is applicable to an emission from a single grid cell or to a complete 2D emission field; i.e. E_X and $E_{X,s}$ may be 2D fields. The functions may further depend on the country of the source. In that case, a further summation over countries is needed in combination with country masks. Our Python package and online emission module support country-specific time functions.

The generated netCDF files contain time functions of diurnal, day-of-week and seasonal variations per tracer and source category. These scalings are provided in three separate files by default. However, it is also possible to provide only one file with hour-of-year scaling factors. The temporal profile variables are arrays with the two dimensions time (e.g. 24 different hours of day in case of a diurnal profile) and country. If no country-specific information is available or desired, a uniform country mask with a single value for the whole model domain needs to be generated. Vertical profiles, in contrast, are 1D arrays with level as the only dimension, since they are not expected to vary with country.

With this approach, real trace gases such as CO_2 can be simulated but also idealized tracers representing only a subset of sources, for example a tracer representing only traffic CO_2 emissions, by only summing over a subset of source categories in Eq. (3).

Emissions do not only occur at the surface but should be treated in 3D (Bieser et al., 2011b; Brunner et al., 2019). This is particularly true for elevated emissions from power plants or air traffic. Idealized vertical scaling functions v_s are available for anthropogenic emissions, which distribute the emissions from a source of category s over a discrete set of geometric vertical layers (altitude relative to ground). The scaling factors add up to 1 when summed over all vertical layers. Examples are given in the Supplement. The emission of the simulated tracer X at time t and in vertical layer k is then given as

$$E_{X,k}(t) = \sum_{s=0}^n E_{X,s} \cdot w_{X,s}(t) \cdot v_{X,s,k}. \quad (4)$$

The **vertical-profiles** file generated by the Python tool contains vertical profiles per tracer and source category. The number of levels and their heights above surface can be set independently of the vertical structure of the COSMO grid. The vertical profiles do not depend on time t in the current implementation of the module. This could be implemented in the future, for example to account for meteorology-dependent plume rise of emissions from power plants.

2.4 Speciation

The chemical compounds simulated in COSMO-ART include species for which inventories provide direct emission strengths (e.g. SO_2 or NH_3). However, for other species, the inventories only provide aggregated information for a family of compounds. This is the case for NO_x (sum of NO and NO_2), NMVOCs, and particulate matter with a diameter of less than $2.5 \mu\text{m}$ ($\text{PM}_{2.5}$) and $10 \mu\text{m}$ (PM_{10}) (sum of various organic and inorganic aerosol compounds).

Therefore, to compute the emission of an individual compound simulated in the model, chemical speciation factors have to be applied to the total mass of the family. These speciation factors are specific for different source categories, since, for example, the composition of NMVOCs, PM and NO_x emissions is different for traffic and residential heating. Furthermore,

the speciation factors depend on the specific chemical mechanism applied in the model, which determines the mapping between real and model-simulated species.

Starting from Eq. (4), considering a simulated tracer X whose emissions are reported under a chemical compound \tilde{X} with a speciation factor $f_{\tilde{X} \rightarrow X}$ (dimensionless), the emission of ~~species X~~ at vertical level k ~~additionally accounting for source~~

5 ~~speciation factor f~~ is given by

$$E_{X,k}(t) = \sum_{s=0}^n E_{\tilde{X},s} \cdot f_{\tilde{X} \rightarrow X,s} \cdot w_{X,s}(t) \cdot v_{X,s,k}. \quad (5)$$

2.5 Mapping to COSMO-grid

~~All emission data need to be mapped onto the simulation grid, which in case of COSMO is a rotated latitude-longitude grid. Such a mapping is not trivial, since simple interpolation is not mass-conservative, whereas conservative nearest neighbor methods may lead to undesired stripes or other discontinuities. In order to avoid such issues and to accurately conserve mass, we determine for each grid cell of the inventory the cells of the COSMO-grid intersecting it, compute the areas of intersection, and store the ratios between intersected and total area of the cell. Finally, for each model grid cell, the emission contributions of all computed intersections weighted by the corresponding ratios are summed up. A minor caveat is that the area of intersection is computed in degree² instead of true geometric areas. We found this to be an acceptable approximation with errors of less than 0.1% for inventory grid cells of dimension 0.1° x 0.1° at up to 60° latitude.~~

3 Implementation in COSMO-GHG and COSMO-ART

The online module was implemented in two extended versions of COSMO, COSMO-GHG developed for the simulation of passive tracers (e.g. greenhouse gases), and COSMO-ART for reactive trace gases and aerosols. An early version of the COSMO-GHG extension was developed in the CarboCount-CH project (Liu et al., 2017). It was built atop a generic tracer module, which was introduced in COSMO version 5.0 to enable a flexible definition of tracers with specific properties defined by their metadata (Roches and Fuhrer, 2012). In the standard weather prediction version of COSMO it is used for the advective, convective and turbulent transport of all moisture tracers (water in the gas phase and in different hydrometeor phases). However, the life cycle of a tracer usually involves also other aspects not considered in COSMO such as emissions or removal from the atmosphere. In the GHG extension, emissions can be supplied in the form of 2D surface fluxes or 3D volume emissions.

25 To activate the GHG extension, COSMO has to be compiled with the `-DGHG` flag to enable the `#ifdef GHG` directives. Table 1 summarizes those interfaces to the GHG extension, including subroutine calls and number of `#ifdef` directives in the COSMO code.

Recently, the standard, CPU-based (Central Processing Unit) COSMO version released by the German Weather Service has been fully ported to GPUs (Graphics Processing Unit) (Fuhrer et al., 2014). This efficient GPU-enabled code, called COSMO-POMPA (Performance On Massively Parallel Architectures), is used operationally by the Swiss Federal Office of Meteorology and Climatology (MeteoSwiss) for daily weather forecasting. COSMO-POMPA has been integrated into the ~~latest-official~~

Table 1. Changes due to the GHG extension in the COSMO code

File name	Description	No. of ifdefs	Remarks
m_online_emissions.f90 <u>m_online_emissions.f90</u>	Contains subroutines for the reading in and computation of the gridded emissions vertical and temporal profiles for the online anthropogenic emissions module.	-	New file
acc_global_data.f90 <u>acc_global_data.f90</u>	Performs allocation/deallocation of global fields on the accelerator using OpenACC directives.	2	1 subroutine ca
data_io.f90 <u>data_io.f90</u>	Contains all data necessary for input and output of grib or netCDF files.	1	2 additional va
lmorg.f90 <u>lmorg.f90</u>	Main program.	6	8 subroutine ca
organize_data.f90 <u>organize_data.f90</u>	Organizes the I/O of the model.	5	7 subroutine ca

~~COSMO-release-5.6a~~ official version of COSMO since its release 5.5b, which can be compiled for both CPU- und GPU-based systems.

In order to benefit from the high efficiency of the GPU-enabled code, the GHG extension was ported to GPUs in the framework of the project SMARTCARB (Brunner et al., 2019). The porting was done using OpenACC compiler directives, which is a high-level approach to offload compute-intensive parts to a GPU accelerator (Lapillonne and Fuhrer, 2014). The same approach was employed for the porting of the online emission module. ~~Since COSMO~~ COSMO-GHG is available for COSMO version 5.6a and it is planned to be integrated continuously for all upcoming releases of COSMO. Since COSMO 5.6a can be compiled for both CPU- and GPU-based platforms, the GHG-extension and the online emission module had to be programmed in a way that they can be executed on both platforms as well. Depending on the chosen platform, code sections related to OpenACC directives are included or excluded from compilation based on `#ifdef _OPENACC` compiler directives.

COSMO-ART was developed at the Karlsruhe Institute of Technology for the simulation of air pollutants and their interactions with meteorology (Vogel et al., 2009; Knote et al., 2011). The ART extension makes use of the same generic tracer mechanism implemented in COSMO, but adds an additional layer (a structure `art_species`) allowing for a more comprehensive definition of tracer properties such as molecular weight, initial and boundary values, deposition properties and so on. For each ART species, a corresponding tracer is generated and dynamically allocated in memory. The position of the associated tracer is referenced by an index in the `art_species` structure. Because the ART extension has not yet been ported to GPUs, COSMO-ART does not run with COSMO 5.6a but with an older release 5.1.

3.1 Basic framework for online emission processing in COSMO

The main philosophy is to read in all input data required for the online emission module only once at the start of the simulation. These data include annual mean sector-specific 2D emission fields $E_{X,s}$ as well as the temporal, vertical and speciation profiles.

Table 2. Members of the GHGCTL and OAECTL namelist group required in INPUT_GHG for COSMO-GHG and INPUT_OAE for COSMO-ART, respectively, for setting up the online emission module.

Name	Description	Variable type
in_tracers	Number of TRACER groups (see Table 2.3)	INT
vertical_profile_nc	Filename for vertical profiles	CHAR
hour_of_day_nc	Filename for “ hour-of-day hour-of-day” time profiles	CHAR
day_of_week_nc	Filename for “ day-of-week day-of-week” time profiles	CHAR
month_of_year_nc	Filename for “ month-of-year month-of-year” time profiles	CHAR
hour_of_year_nc	Filename for “ hour-of-year hour-of-year” time profiles	CHAR
gridded_emissions_nc	Filename for gridded emissions	CHAR
iemiss_interp	Type of temporal interpolation (only COSMO-GHG) 0: constant emissions read for present full hour 1: linear interpolation of emissions between present and next full hour	INT

Table 3. Namelist members of the TRACER group in INPUT_GHG and INPUT_OAE, respectively. Some namelist members are only implemented in COSMO-GHG or COSMO-ART.

Name	Description	Variable type	Default value
yshort_name	Name of tracer	CHAR	‘undefined’
itype_emiss	Type of 3D volume emissions (only COSMO-GHG): 0: no emissions 1: offline emissions (i.e., read from file) 2: online emissions	INT	−999
itype_tscale	Type of temporal scaling (only COSMO-GHG) 0: no temporal scaling 1: temporal scaling using hour-of-day, day-of-week and month-of-year <u>hour-of-day, day-of-week and month-of-year</u> 2: temporal scaling using hour-of-year <u>hour-of-year</u>	INT	0
ycatl(:)	List of categories <i>s</i> considered as sources of the tracer	CHAR	-
ytpl(:)	List of temporal profiles used for each element of ycatl	CHAR	-
yvpl(:)	List of vertical profiles used for each element of ycatl	CHAR	-
contribl(:)	List of speciation factors per category (only COSMO-ART)	REAL	−10.0

During the simulation, these profiles are applied online to update the hourly emissions for each species according to ~~equations 2-5~~Eqs. (2)-(5).

In order to implement new tracers flexibly, TRACER groups were added to the INPUT_GHG namelist file. A subset of the possible entries (members) of the TRACER group is presented in Table ??3 and an example ~~with a complete list of entries~~ namelist file is given in the Supplement. For the online emission module, the definition of the TRACER group was extended with the following parameters:

- 5 1. A new possible value for the switch `itype_emiss`, which needs to be set to 2 to activate online emissions for this tracer.
2. A list tag `ycatl` listing the categories s considered as sources of the tracer.
3. A list tag `ytpl` listing the temporal profile used for each element of `ycatl`.
4. A list tag `yvpl` listing the vertical profile used for each element of `ycatl`.
- 10 5. A list tag `contribl` used for chemical speciation, which lists the contribution of categories s to the total emitted mass of the tracer (only COSMO-ART).

Note that the comma-separated lists `ycatl`, `ytpl`, `yvpl` and `contribl` need to have the same length. In contrast to COSMO-GHG, the definition of tracers is fixed (i.e. hard-coded) in COSMO-ART and, therefore, no namelist file INPUT_GHG exists. In order to enable the same functionality as in COSMO-GHG, a new namelist file INPUT_OAE was introduced, where
15 for each emitted tracer a corresponding TRACER group has to be defined (OAE = Online Anthropogenic Emissions). In order to enable or disable the use of online emissions in COSMO-ART, a new boolean switch `lemiss_online` was implemented in the namelist file INPUT_ART, which needs to be set to `.TRUE.` to activate the online emission module. For this reason, the namelist switch `itype_emiss` does not exist in COSMO-ART. The same applies for `itype_tscale`, since temporal scaling is applied just for hour-of-day, day-of-week and month-of-year profiles.

- 20 At the start of a simulation, the online emission module reads in the emission fields and the temporal and vertical profiles from the ~~following~~ netCDF files generated by the Python tool (full-, which have been described in Sect. 2. Full paths of the files have to be specified in the namelist file INPUT_GHG or INPUT_OAE, see Table ??): ~~gridded_emissions_nc: 2D gridded fields $E_{X,s}$ of tracers X for all source categories s contributing to emissions of X directly on the COSMO grid. The netCDF variable names need to be identical to the category names s listed in `ycatl`. This file also contains a corresponding~~
25 ~~2D country mask, which is an integer field with each grid cell being assigned the number of the country that has the largest fractional area. `hour_of_day_nc`, `day_of_week_nc`, `month_of_year_nc`: Time functions of diurnal, day-of-week and seasonal variations per tracer and source category. These scalings are provided in three separate files by default. However, it is also possible to provide only one file `hour_of_year_nc`~~ 2. Note that variable names within the netCDF files have to be identical with ~~hour-of-year scaling factors by setting `itype_tscale` to 2. The netCDF variable names must be identical~~
30 ~~to those listed in the `ycatl`, `ytpl` list for each category s . `vertical_profile_nc`: Vertical profiles per tracer and source category. The number of levels and their heights above surface can be set independently of the vertical structure of the COSMO grid. The netCDF variable names need to be identical to those listed in the `yvpl` list for each category s , as shown in Table 4.~~

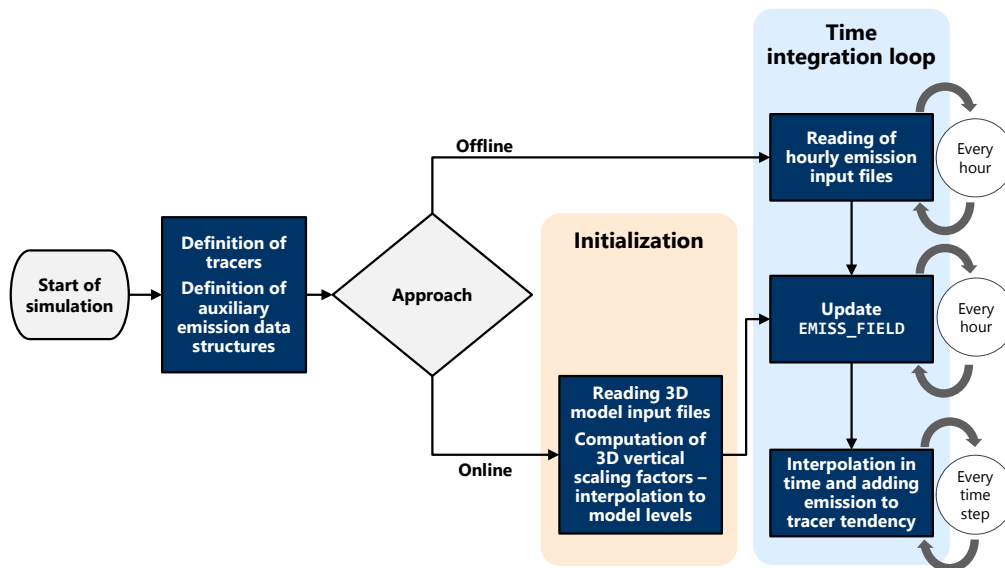


Figure 2. Flow chart for COSMO-GHG run-time processes both for the offline and online approach. Blue rectangles are code parts. The simulation start point is represented by an oval.

Table 4. Overview of netCDF files and corresponding namelist tags in the TRACER group in INPUT_GHG or INPUT_OAE. The netCDF variable names must be identical to those listed in the namelist members (right column).

<u>Variable for netCDF file name</u>	<u>Namelist member</u>
<u>gridded_emissions_nc</u>	<u>ycatl</u>
<u>hour_of_day_nc</u>	<u>ytpl</u>
<u>day_of_week_nc</u>	<u>ytpl</u>
<u>month_of_year_nc</u>	<u>ytpl</u>
<u>hour_of_year_nc</u>	<u>ytpl</u>
<u>vertical_profile_nc</u>	<u>yvpl</u>

Temporal profiles are arrays with the two dimensions time (e.g. 24 different hours of day in case of a diurnal profile) and country. If no country-specific information is available or desired, a uniform country mask with a single value for the whole model domain needs to be generated. Vertical profiles, in contrast, are 1D arrays with level as the only dimension, since they are not expected to vary with country.

- Speciation profiles for COSMO-ART are not provided in a separate netCDF file but are included in the namelist file INPUT_OAE through the list tag contribl of the TRACER group.

3.2 Modifications to the COSMO-GHG and COSMO-ART codes

In order to enable the computation of online emissions as an alternative to the default offline reading of emission files, the greenhouse gas module of COSMO-GHG (`m_online_emissions.f90`) was extended with new structures to store the information on temporal and vertical profiles and the annual mean sectorial emission grids. The arrays for temporal profiles and the emission grids are dynamically allocated as they depend on the tracer type. The information from the netCDF files is read at the beginning of the simulation. The vertical scaling factors, which are defined for layers above ground of fixed vertical extent (see Supplement), need to be translated into scaling factors for the vertical layers of COSMO. Since COSMO uses a spatially fixed grid with geometric hybrid vertical layers with thicknesses varying with the underlying topography, the vertical scaling factors are translated into dynamically allocated 3D arrays.

Before the implementation of the online emission module in COSMO-GHG, emissions were read in every hour from a file and assigned to an emission field associated with each tracer. In COSMO-GHG, fields that are conceptually attached to a prognostic variable of the model (e.g. an emission field attached to a tracer) are called associated fields. The definition, memory management and I/O aspects of associated fields are handled in `src_associated_fields.f90`. There, besides the already existing functionality of reading in files, a mechanism was added to compute the emissions based on the dynamically allocated arrays for the emission grid and temporal and vertical scaling factors. Afterwards, no matter if online or offline emissions are used, the emission fields are updated at the beginning of each hourly interval. The updates account for the new temporal scaling for the current hour and the 3D vertical scaling factors calculated at the beginning of the simulation by applying Eq. (4). The emissions are then kept constant during the current hour or linearly interpolated in time between the current and the next hour (if `iemiss_interp` is set to 1). The latter requires the computation (or reading) of the emission field at the following full hour. Finally, the emission field is added to the tracer tendencies at each model time step. All relevant computations in the GHG module use OpenACC directives in a similar manner as in other parts of the main COSMO code. A schematic of all relevant processes for offline and online emissions in COSMO-GHG during model run-time is shown in Fig. 2.

Even though the concepts are very similar, the realization of the online emission module in COSMO-ART differed significantly from the implementation in COSMO-GHG. The emission module in ART (`art_emiss_prescribed.f90`) comes on top of the tracer module in COSMO and interacts closely with the tracer fields in other ART modules such as `art_mademod.f90` for aerosol processes. It was therefore desirable to keep most of the functionality of the standard emission modules to ensure the usability of both online and offline emission versions. The online emission module in COSMO-ART works as follows, focusing on the differences to the COSMO-GHG implementation: During initialization of the model, if the namelist parameter `lemiss_online` is set to `.TRUE.`, the required files (emissions, temporal and vertical scaling factors) are read in as described in Sect. 3.1. For every tracer with online emissions, the gridded emissions, the scaling factors (temporal and vertical), as well as speciation values, are collected in a data structure that associates this information with the location of that tracer in the `art_species` structure. Then, at hourly intervals during the run, the emissions are calculated and written into the corresponding array in `art_species`. Because this replaces the assignment of emissions read in from external files

to the same array as done in the standard offline version, no further changes to other modules are required. It is even possible to mix on- and offline emissions in a simulation run, such that emissions of certain tracers are read in, while others are calculated.

3.3 Practical examples

3.3.1 Merging of inventories

- 5 For regional scale simulations it is often desired to merge different inventories covering different regions, e.g. nesting the high-resolution Swiss national inventory into the coarser European inventory of TNO. Two different approaches have been implemented in the Python tool to tackle this use-case. For both approaches, the different inventories have to be mapped individually to the model grid using the Python tool as a first step. Afterwards, the inventories may be merged using a country mask by overwriting the data of the coarser inventory with the data from the high-resolution one for all grid cells corresponding
- 10 to the selected country (or region). A simpler approach is to make use of the fact that temporal profiles can be country-specific. To merge the two inventories during the online processing, the `hourofday` profile for the coarse inventory can be set to 0 for the country covered by the high-resolution inventory and vice versa for the high-resolution inventory.

3.3.2 Distinction between area and point source emissions

- The inventories of TNO differentiate between area and point source emissions. Point source emissions as reported to the
- 15 European Pollutant Release and Transfer Registry (E-PRTR) correspond to strong local sources, which are often emitted from tall stacks. An example is emissions from residential heating, which can originate from large centralized facilities (possibly reported to E-PRTR) or from individual houses (reported as area sources). It may be desirable to apply different temporal and vertical profiles to these different types of sources. The Python tool allows generating separate grid maps and temporal and vertical profiles for point and area sources. Using these different maps and profiles for a given tracer is then straightforward,
- 20 since point and area sources can be treated like separate source categories that need to be listed in the `ycatl`, `ytpl`, and `yvpl` tags of the tracer namelist group.

3.3.3 Modification of temporal and chemical speciation profiles

- In a study of Athanasopoulou et al. (2017), the effect of the financial crisis in Greece on domestic fuel use and air pollution was investigated as an air quality modeling study using COSMO-ART. Due to the financial crisis, there was a sharp increase
- 25 in wood burning for residential heating, which had major implications for air quality in Athens. Based on measurements of black carbon in the city, it became clear that the standard temporal profiles had to be updated to better reflect the actual burning of wood. For example, the standard profiles for residential heating predicted peaks of similar amplitude in the morning and evening and a minimum during weekends. This largely contrasted with the measurements which suggested maximum usage during weekends and a major peak in the evening but not in the morning. Furthermore, the speciation of PM_{2.5} emissions had
- 30 to be modified, since wood burning emissions contain a large proportion (approx. 80%) of primary organic aerosols. Adjusting the temporal and speciation profiles required changes to the emission pre-processing software and regenerating all hourly input

files for the simulation. Using the online emission module, the same could have been achieved by a simple replacement of the temporal profiles in the netCDF files and of the speciation profiles in the namelist file `INPUT_OAE`.

4 Performance evaluation (offline vs. online emissions)

Two sets of simulations comparing the results of online and offline emission handling using COSMO-GHG and COSMO-ART, respectively, are presented in the following. The comparison is made in terms of performance (computation time and storage requirements) and in terms of simulated tracer fields. Ideally, the two approaches should lead to identical results, but as will be shown, small numerical errors e.g. due to truncation of floating point numbers were found to produce small differences.

4.1 COSMO-GHG

Using the COSMO-GHG model with online and offline setup, respectively, a simulation with a single CO_2 tracer for a domain covering the Alpine region at $0.01^\circ \times 0.01^\circ$ (≈ 1.1 km) horizontal resolution and with 60 vertical levels was conducted. The simulation extended over a period of one week from 1 January 2019 to 8 January 2019. The boundary conditions for meteorological fields were taken from COSMO-7 reanalyses provided by MeteoSwiss. The CO_2 tracer field was initialized to 0.

The model setup closely followed the settings of the operational high-resolution COSMO-1 forecast of MeteoSwiss. The simulations were performed on 60 hybrid CPU-GPU nodes of the Piz Daint supercomputer of the Swiss National Supercomputing Centre (CSCS). Each node included an Intel Xeon E5-2690 v3 12-core CPU and an NVIDIA Tesla P100 GPU.

The yearly gridded anthropogenic emissions of CO_2 were taken from the TNO-GHGco inventory for 2015 available at $0.1^\circ \times 0.05^\circ$ resolution. They were split into 12 GNFR categories. The F category for road transport was further divided in 3 subcategories depending on the type of vehicles. Over Switzerland, the TNO inventory was replaced by a Swiss CO_2 inventory at $500\text{ m} \times 500\text{ m}$ resolution, which was created by the company MeteoTest in the framework of the CarboCount-CH project (Liu et al., 2017). Due to a different source categorization used in the Swiss inventory, those categories were mapped to the GNFR categories B, C, F, J and L. The temporal profiles applied to the emissions are described in the Supplement. No vertical profiles were applied in this example, but all emission were released at the surface. The namelist definition of the tracer in this simulation is described in the Supplement.

An example of the distribution of the simulated CO_2 tracer representing all anthropogenic emissions in the domain and of the differences between online and offline is shown in Fig. 3. The figure shows instantaneous near-surface CO_2 at the end of the 7-day simulation period.

The differences between online and offline are negligible (around 10^{-6} ppm) almost everywhere except for a plume in southern Germany. This difference can be explained by a point source in the TNO inventory, which is located exactly on the border of a COSMO grid cell. When generating online and offline emissions, two separate gridded maps of emissions need to be produced.¹ Because of floating point truncation errors, this point source was attributed to two adjacent grid cells when

¹This is due to the fact that offline emissions are later pre-processed through `int2lm`, which requires a slightly larger domain.

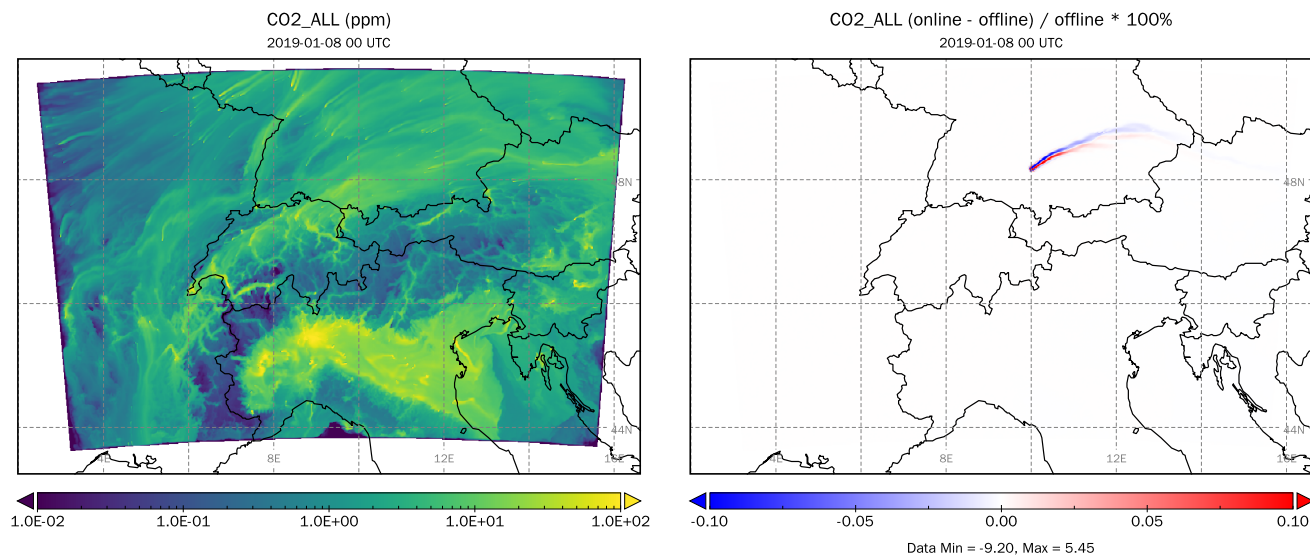


Figure 3. Surface-layer concentrations for the online simulation (left) and relative differences between online and offline simulations (right) of the CO₂ tracer corresponding to all anthropogenic emissions after seven days in the COSMO-GHG test case.

processed with the online and offline approach. The spatial shift of this plume leads to differences of around ± 0.15 ppm but the spatial mean remains almost constant (differs less than 10^{-7} ppm).

In terms of computation time the two COSMO-GHG runs were almost identical, as seen in Table ??5. Disk usage, on the other hand, was dramatically reduced when using online emissions (about 3% of the offline case). This benefit would have been even larger for a longer simulation period. Furthermore, the time consumption for generating the online input files is more than halved compared to the hourly offline files, as shown in Table 6.

4.2 COSMO-ART

The online and offline emission approaches of COSMO-ART were compared by performing a test simulation over Europe with a horizontal resolution of $0.12^\circ \times 0.12^\circ$ (≈ 13 km) and 60 vertical levels. The simulation was driven by meteorological fields from the European Centre for Medium-Range Weather Forecasts (ECMWF) Integrated Forecast System (IFS) model. The initial and boundary conditions for the chemical species were taken from the global MOZART-4 model (Emmons et al., 2010). A standard configuration with RADMK chemical mechanism, Volatility Basis Set (VBS) for organic aerosols and ISORROPIA-II scheme for inorganic aerosols was selected as described in Athanasopoulou et al. (2013). The configuration for the meteorology closely followed the setup of the operational European COSMO-7 forecasts of MeteoSwiss. The 24 h test simulation was started at 26 June 2015, 00 UTC and ended at 27 June 2015, 00 UTC. It was conducted on 16 CPU nodes of Piz Daint. Each node consisted of two Intel Xeon E5-2695 v4 processors providing a total of 36 cores per node. The simulation thus used a total of 576 cores.

Table 5. Simulation time and input data size for online and offline COSMO-GHG and COSMO-ART test cases.

	Online	Offline	Online / Offline
COSMO-GHG <i>COSMO-GHG (7-day simulation)</i>			
Simulation time	3 h 49 min	3 h 57 min	0.96
Input size	80 MB	2800 MB	0.03
COSMO-ART <i>COSMO-ART (1-day simulation)</i>			
Simulation time	19 min 34 s	19 min 47 s	0.99
Input size	59 MB	5600 MB	0.01

The European anthropogenic emission inventory CAMS-REG-AP_v2_2 ([Granier et al., 2019](#)) generated by TNO was combined with the Swiss national emission inventory for reactive gases and aerosols generated by Meteotest Inc. Both inventories were based on the GNFR source classification. The two inventories were merged using a country mask for Switzerland, i.e., following the first approach described in [Section Sect. 3.3.1](#).

5 The COSMO-ART simulations with online and offline emissions have almost identical outputs for the same test simulation as shown in Fig. 4 for surface-layer concentrations of the gas phase species SO₂ and ethane and for particulate sulfate (SO₄, variable `VS04J` in COSMO-ART). The differences for SO₂ and ethane are in the order of numerical noise. For SO₄ the differences are larger but still several orders of magnitude smaller than the absolute concentrations. Due to the complexity and non-linearity of aerosol chemistry within COSMO-ART, small differences may eventually build up in the course of the simulation. While maximum relative differences of SO₄ are up to 10% for a few grid points, the spatial mean of these differences are small with 0.044%. Further statistical values for SO₄ and other variables are provided in the Supplement.

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Similar to COSMO-GHG, the computation time was quite comparable for the two versions, as seen in [Table?? 5](#). The reduction in time spent on I/O in the online version is thus largely compensated by the increase in computation time. Disk usage for the online emission version was only about 1% of the usage for the offline version. Again, the benefit in disk usage would grow proportionally with increasing length of the simulation period.

15

5 Conclusions

A comprehensive online emission processing tool for atmospheric composition simulations was presented and demonstrated for two atmospheric transport models, COSMO-GHG and COSMO-ART. The tool is composed of a standalone Python package as well as a model-specific Fortran 90 module, which was integrated into the two models. The Python tool prepares the input for the simulation (a small set of netCDF files), which consists of gridded emission maps per source category (projected to the model grid), and temporal and vertical emission profiles. The Fortran 90 module reads these inputs at the beginning of a simulation and updates the 3D emissions for each simulated tracer at regular (e.g. hourly) intervals taking into account the

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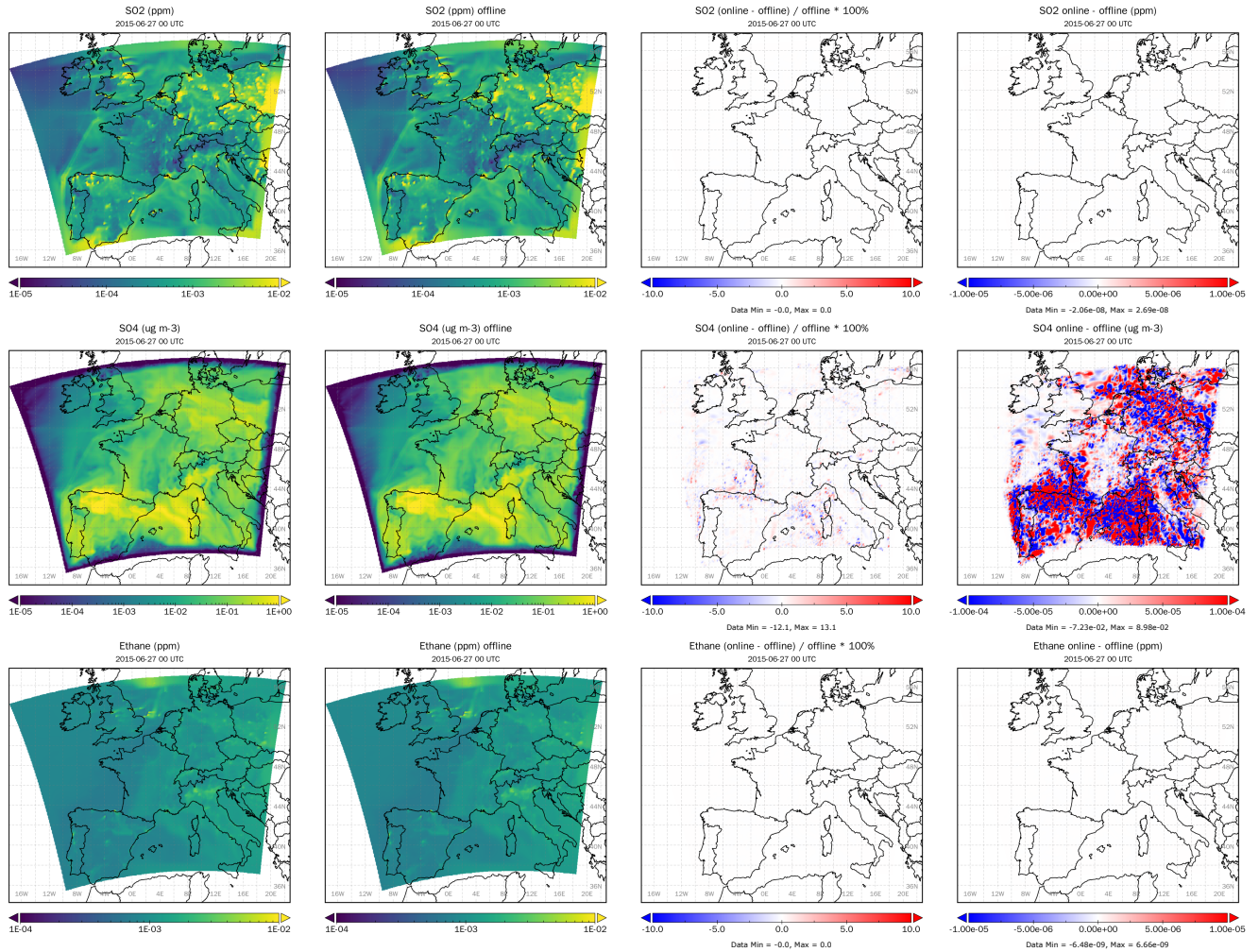


Figure 4. Surface-layer concentrations for the online and offline simulations, relative and absolute differences between online and offline simulations in the COSMO-ART test case for surface layer fields of SO_2 (atop) SO_2 , SO_4 (bmiddle) SO_4 and ethane (ebottom) ethane -after 24 h.

corresponding temporal and vertical emission profiles. For COSMO-ART, additional speciation profiles have to be provided to distribute the emissions of a family of compounds like NMVOC over the individual model species.

The Python package is independent of the specific model implementation and is also able to generate hourly emission fields for models using the traditional offline approach. The Fortran 90 module, in contrast, was specifically designed for the two
5 COSMO variants and will have to be adapted for other model systems.

The online approach greatly simplifies the setup of new model simulations, since a single set of a few input files is sufficient for all simulations on a given model grid irrespective of the simulated time period. In comparison to the offline approach,

Table 6. Benchmark for pre-processing online and offline emissions for the COSMO-GHG test case using the emiproc tool. Altogether, 19 categories from the emission inventories were processed (TNO: 14, Swiss: 5) as input for the CO₂ tracer. Pre-processing was performed on a local Linux cluster, using 14 threads in parallel. Processing times for generating the mapping and country mask files are excluded. Results are shown for different dataset lengths.

Processing step	Processing time (s)		
	1 day	7 days	365 days
Mapping and merging of inventories, creating netCDF files	78	78	78
Offline Processing: extracting data from netCDF files	106	106	106
Offline Processing: generating offline netCDF files	11	74	3859
Total Online	78	78	78
Total Offline	117	180	3965
Ratio Online / Offline	0.67	0.43	0.02

where a large number of emission input files has to be generated for a simulation, this reduces the ~~storage~~-input requirements by orders of magnitude.

The performance of the online and offline approaches was compared in two test simulations conducted with COSMO-GHG and COSMO-ART, respectively. In both cases the total computation time was almost identical, suggesting that the additional time required for computing hourly emissions online within the model could be compensated by the reduced time spent on I/O. The time required for data pre-processing ~~was not analyzed, but was clearly is~~ much lower for the online approach. Both approaches produced almost identical concentration fields demonstrating their equivalence, with tiny differences attributable to floating point truncation errors.

The online emission approach was successfully introduced in all our COSMO-based model systems and, owing to its flexibility and reduced ~~storage~~-input and data pre-processing requirements, greatly simplified our daily working procedures. The Python package is a valuable tool on its own, as it is independent of the specific model system, can be applied in combination with several popular emission inventories, and offers an accurate mass-conserving method for mapping emissions to a given model grid.

Our tool is tailored to the processing of anthropogenic emissions, which follow a regular pattern in space and time, but it is not suitable for the processing of highly variable emissions such as emissions from biomass burning. This will require an extension to support a combination of offline inputs and online computation. Future developments will focus on the porting to other model systems such as ICON-ART and on the implementation of meteorology-dependent emissions such as those from residential heating or from lightning.

Code and data availability. The Python package “emiproc” for emission pre-processing is publicly available through the C2SM GitHub organization (<https://github.com/C2SM-RCM/cosmo-emission-processing>). The repository also includes the vertical and temporal profiles used here. The emission inventories are not part of the repository. The EDGAR inventory is accessible from the European Joint Research Centre (JRC). The TNO inventories can be accessed through the Copernicus product catalogue (<https://atmosphere.copernicus.eu/catalogue>).

- 5 The Swiss national emission inventories are available from the corresponding author upon request. The online emission module has been implemented both in COSMO-GHG and COSMO-ART. Both Fortran modules are available on the C2SM organization on GitHub and can be obtained from the corresponding author upon request. Access to the COSMO code is restricted to COSMO licensees. A free license can be obtained for research use following the procedure described at <http://www.cosmo-model.org/content/consortium/licencing.htm>.

Author contributions. MJ led the writing of the manuscript with contributions from all co-authors and generated the figures. MJ, DO, GK, 10 JMH, and QM jointly developed the Python package. VC, GK, DO, JMH, MJ and KO jointly developed the Fortran modules. DB proposed the idea, surveyed the study and contributed to the writing. QM and MJ conducted the COSMO-ART simulations, JMH the COSMO-GHG simulations.

Competing interests. The authors declare that they have no conflict of interest.

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References

- Athanasopoulou, E., Vogel, H., Vogel, B., Tsimpidi, A. P., Pandis, S. N., Knote, C., and Fountoukis, C.: Modeling the meteorological and chemical effects of secondary organic aerosols during an EUCAARI campaign, *Atmos. Chem. Phys.*, 13, 625–645, <https://doi.org/10.5194/acp-13-625-2013>, 2013.
- 5 Athanasopoulou, E., Speyer, O., Brunner, D., Vogel, H., Vogel, B., Mihalopoulos, N., and Gerasopoulos, E.: Changes in domestic heating fuel use in Greece: effects on atmospheric chemistry and radiation, *Atmospheric Chemistry and Physics*, 17, 10597–10618, <https://doi.org/10.5194/acp-17-10597-2017>, <https://www.atmos-chem-phys.net/17/10597/2017/>, 2017.
- Baklanov, A., Schlünzen, K., Suppan, P., Baldasano, J., Brunner, D., Aksoyoglu, S., Carmichael, G., Douros, J., Flemming, J., Forkel, R., Galmarini, S., Gauss, M., Grell, G., Hirtl, M., Joffe, S., Jorba, O., Kaas, E., Kaasik, M., Kallos, G., Kong, X., Korsholm, U., Kurganskiy, A., Kushta, J., Lohmann, U., Mahura, A., Manders-Groot, A., Maurizi, A., Moussiopoulos, N., Rao, S. T., Savage, N., Seigneur, C., Sokhi, R. S., Solazzo, E., Solomos, S., Sørensen, B., Tsegas, G., Vignati, E., Vogel, B., and Zhang, Y.: Online coupled regional meteorology chemistry models in Europe: current status and prospects, *Atmos. Chem. Phys.*, 14, 317–398, <https://doi.org/10.5194/acp-14-317-2014>, 2014.
- 10 Baldauf, M., Seifert, A., Forstner, J., Majewski, D., Raschendorfer, M., and Reinhardt, T.: Operational convective-scale numerical weather prediction with the COSMO model: description and sensitivities, *Monthly Weather Review*, 139, 3887–3905, <https://doi.org/10.1175/MWR-D-10-05013.1>, 2011.
- 15 Bieser, J., Aulinger, A., Matthias, V., Quante, M., and Builtjes, P.: SMOKE for Europe - adaptation, modification and evaluation of a comprehensive emission model for Europe, *Geoscientific Model Development*, 4, 47–68, <https://doi.org/10.5194/gmd-4-47-2011>, <https://www.geosci-model-dev.net/4/47/2011/>, 2011a.
- 20 Bieser, J., Aulinger, A., Matthias, V., Quante, M., and van Der Gon, H. D.: Vertical emission profiles for Europe based on plume rise calculations, *Environmental Pollution*, 159, 2935–2946, <https://doi.org/10.1016/j.envpol.2011.04.030>, <http://www.sciencedirect.com/science/article/pii/S0269749111002387>, 2011b.
- Borge, R., Lumberras, J., and Rodr guez, E.: Development of a high-resolution emission inventory for Spain using the SMOKE modelling system: A case study for the years 2000 and 2010, *Environmental Modelling & Software*, 23, 1026 – 1044, <https://doi.org/https://doi.org/10.1016/j.envsoft.2007.11.002>, <http://www.sciencedirect.com/science/article/pii/S1364815207002174>, 2008.
- 25 Brunner, D., Kuhlmann, G., Marshall, J., Cl ment, V., Fuhrer, O., Broquet, G., L scher, A., and Meijer, Y.: Accounting for the vertical distribution of emissions in atmospheric CO₂ simulations, *Atmospheric Chemistry and Physics*, 19, 4541–4559, <https://doi.org/10.5194/acp-19-4541-2019>, <https://www.atmos-chem-phys.net/19/4541/2019/>, 2019.
- 30 Centre on Emission Inventories and Projections (CEIP): User guide to WebDab, https://www.ceip.at/ms/ceip_home1/ceip_home/webdab_emepdatabase/webdab_usersguide/, last access: 2019-07-10, 2018.
- Crippa, M., Guizzardi, D., Muntean, M., Schaaf, E., Dentener, F., van Aardenne, J. A., Monni, S., Doering, U., Olivier, J. G. J., Pagliari, V., and Janssens-Maenhout, G.: Gridded emissions of air pollutants for the period 1970–2012 within EDGAR v4.3.2, *Earth System Science Data*, 10, 1987–2013, <https://doi.org/10.5194/essd-10-1987-2018>, <https://www.earth-syst-sci-data.net/10/1987/2018/>, 2018.
- 35 Denier van der Gon, H., Hendriks, C., Kuenen, J., Segers, A., and Visschedijk, A.: Description of current temporal emission patterns and sensitivity of predicted AQ for temporal emission patterns: TNO Report, EU FP7 MACC deliverable report D_D-EMIS_1.3, Report, MEP-R2003/166, Apeldoorn, The Netherlands, 2011.

- EEA: EMEP/CORINAIR Atmospheric emission inventory guidebook - Second edition 1999, Report, <https://www.eea.europa.eu/publications/EMEPCORINAIR/>, 2000.
- Emmons, L. K., Walters, S., Hess, P. G., Lamarque, J.-F., Pfister, G. G., Fillmore, D., Granier, C., Guenther, A., Kinnison, D., Laepple, T., Orlando, J., Tie, X., Tyndall, G., Wiedinmyer, C., Baughcum, S. L., and Kloster, S.: Description and evaluation of the Model for Ozone and Related chemical Tracers, version 4 (MOZART-4), *Geoscientific Model Development*, 3, 43–67, <https://doi.org/10.5194/gmd-3-43-2010>, <https://www.geosci-model-dev.net/3/43/2010/>, 2010.
- Freitas, S. R., Longo, K. M., Alonso, M. F., Pirre, M., Marecal, V., Grell, G., Stockler, R., Mello, R. F., and Sánchez Gácita, M.: PREP-CHEM-SRC - 1.0: a preprocessor of trace gas and aerosol emission fields for regional and global atmospheric chemistry models, *Geoscientific Model Development*, 4, 419–433, <https://doi.org/10.5194/gmd-4-419-2011>, <https://www.geosci-model-dev.net/4/419/2011/>, 2011.
- 10 Fuhrer, O., Osuna, C., Lapillonne, X., Gysi, T., Cumming, B., Bianco, M., Arteaga, A., and Schulthess, T.: Towards a performance portable, architecture agnostic implementation strategy for weather and climate models, *Supercomput. Front. Innov.: Int. J.*, 1, 45–62, <https://doi.org/10.14529/jsfi140103>, 2014.
- Glassmeier, F., Possner, A., Vogel, B., Vogel, H., and Lohmann, U.: A comparison of two chemistry and aerosol schemes on the regional scale and the resulting impact on radiative properties and liquid- and ice-phase aerosol–cloud interactions, *Atmospheric Chemistry and Physics*, 17, 8651–8680, <https://doi.org/10.5194/acp-17-8651-2017>, <https://www.atmos-chem-phys.net/17/8651/2017/>, 2017.
- 15 Granier, C., Darras, S., Denier van der Gon, H., Doubalova, J., Elguindi, N., Galle, B., Gauss, M., Guevara, M., Jalkanen, J.-P., Kuenen, J., Lioussé, C., Quack, B., Simpson, D., and Sindelarova, K.: The Copernicus Atmosphere Monitoring Service global and regional emissions (April 2019 version), <https://doi.org/10.24380/D0BN-KX16>, https://atmosphere.copernicus.eu/sites/default/files/2019-06/cams_emissions_general_document_apr2019_v7.pdf, 2019.
- 20 Guevara, M., Tena, C., Porquet, M., Jorba, O., and Pérez García-Pando, C.: HERMESv3, a stand-alone multi-scale atmospheric emission modelling framework – Part 1: global and regional module, *Geoscientific Model Development*, 12, 1885–1907, <https://doi.org/10.5194/gmd-12-1885-2019>, <https://www.geosci-model-dev.net/12/1885/2019/>, 2019.
- Janssens-Maenhout, G., Crippa, M., Guizzardi, D., Muntean, M., Schaaf, E., Dentener, F., Bergamaschi, P., Pagliari, V., Olivier, J. G. J., Peters, J. A. H. W., van Aardenne, J. A., Monni, S., Doering, U., and Petrescu, A. M. R.: EDGAR v4.3.2 Global Atlas of the three major Greenhouse Gas Emissions for the period 1970–2012, *Earth System Science Data Discussions*, 2017, 1–55, <https://doi.org/10.5194/essd-2017-79>, <https://www.earth-syst-sci-data-discuss.net/essd-2017-79/>, 2017.
- 25 Keller, C. A., Long, M. S., Yantosca, R. M., Da Silva, A. M., Pawson, S., and Jacob, D. J.: HEMCO v1.0: a versatile, ESMF-compliant component for calculating emissions in atmospheric models, *Geoscientific Model Development*, 7, 1409–1417, <https://doi.org/10.5194/gmd-7-1409-2014>, <https://www.geosci-model-dev.net/7/1409/2014/>, 2014.
- 30 Knote, C., Brunner, D., Vogel, H., Allan, J., Asmi, A., Äijälä, M., Carbone, S., van der Gon, H. D., Jimenez, J. L., Kiendler-Scharr, A., Mohr, C., Poulain, L., Prévôt, A. S. H., Swietlicki, E., and Vogel, B.: Towards an online-coupled chemistry-climate model: evaluation of trace gases and aerosols in COSMO-ART, *Geoscientific Model Development*, 4, 1077–1102, <https://doi.org/10.5194/gmd-4-1077-2011>, <http://www.geosci-model-dev.net/4/1077/2011/>, 2011.
- Kuenen, J. J. P., Visschedijk, A. J. H., Jozwicka, M., and Denier van der Gon, H. A. C.: TNO-MACC_II emission inventory; a multi-year (2003–2009) consistent high-resolution European emission inventory for air quality modelling, *Atmos. Chem. Phys.*, 14, 10 963–10 976, <https://doi.org/10.5194/acp-14-10963-2014>, <http://www.atmos-chem-phys.net/14/10963/2014/>, 2014.

- Lapillonne, X. and Fuhrer, O.: Using Compiler Directives to Port Large Scientific Applications to GPUs: An Example from Atmospheric Science, *Parallel Processing Letters*, 24, 1450 003, <https://doi.org/10.1142/S0129626414500030>, <https://doi.org/10.1142/S0129626414500030>, 2014.
- Liu, Y., Gruber, N., and Brunner, D.: Spatiotemporal patterns of the fossil-fuel CO₂ signal in central Europe: Results from a high-resolution atmospheric transport model, *Atmos. Chem. Phys.*, 2017, 14 145–14 169, <https://doi.org/10.5194/acp-17-14145-2017>, 2017.
- Mailler, S., Menut, L., Khvorostyanov, D., Valari, M., Couvidat, F., Siour, G., Turquety, S., Briant, R., Tuccella, P., Bessagnet, B., Colette, A., Létinois, L., Markakis, K., and Meleux, F.: CHIMERE-2017: from urban to hemispheric chemistry-transport modeling, *Geoscientific Model Development*, 10, 2397–2423, <https://doi.org/10.5194/gmd-10-2397-2017>, <https://www.geosci-model-dev.net/10/2397/2017/>, 2017.
- Matthias, V., Arndt, J. A., Aulinger, A., Bieser, J., van der Gon, H. D., Kranenburg, R., Kuenen, J., Neumann, D., Pouliot, G., and Quante, M.: Modeling emissions for three-dimensional atmospheric chemistry transport models, *Journal of the Air & Waste Management Association*, 68, 763–800, <https://doi.org/10.1080/10962247.2018.1424057>, <https://doi.org/10.1080/10962247.2018.1424057>, PMID: 29364776, 2018.
- McHenry, J. N., Ryan, W. F., Seaman, N. L., Coats, C. J., Pudykiewicz, J., Arunachalam, S., and Vukovich, J. M.: A Real-Time Eulerian Photochemical Model Forecast System: Overview and Initial Ozone Forecast Performance in the Northeast U.S. Corridor, *Bulletin of the American Meteorological Society*, 85, 525–548, <https://doi.org/10.1175/BAMS-85-4-525>, <https://doi.org/10.1175/BAMS-85-4-525>, 2004.
- Pouliot, G., Pierce, T., van der Gon, H. D., Schaap, M., Moran, M., and Nopmongcol, U.: Comparing emission inventories and model-ready emission datasets between Europe and North America for the AQMEII project, *Atmospheric Environment*, 53, 4 – 14, <https://doi.org/https://doi.org/10.1016/j.atmosenv.2011.12.041>, <http://www.sciencedirect.com/science/article/pii/S1352231011013288>, 2012.
- Roches, A. and Fuhrer, O.: Tracer module in the COSMO model, COSMO Technical Report, Report, 2012.
- Schindlbacher, S., Wankmüller, R., and Mareckova, K.: Best practice in gridding emissions — available tools, <https://tfeip-secretariat.org/assets/Meetings/Presentations/Zagreb-2016/Gridding.pdf>, last access: 2019-07-10, 2016.
- United Nations Economic Commission for Europe: Guidelines for Estimating and Reporting Emission Data under the Convention on Long-Range Transboundary Air Pollution/, pp. v, 65 p. ., <http://digitallibrary.un.org/record/517855>, at head of title: Economic Commission for Europe, Geneva., 2003.
- United Nations Economic Commission for Europe: Guidelines for reporting emissions and projections data under the Convention on Long-range Transboundary Air Pollution, <https://www.unece.org/fileadmin/DAM/env/documents/2015/AIR/EB/English.pdf>, last access: 2019-07-10, 2015.
- Vogel, B., Vogel, H., Baumer, D., Bangert, M., Lundgren, K., Rinke, R., and Stanelle, T.: The comprehensive model system COSMO-ART - Radiative impact of aerosol on the state of the atmosphere on the regional scale, *Atmospheric Chemistry and Physics*, 9, 8661–8680, <https://doi.org/10.5194/acp-9-8661-2009>, <GotoISI>://000272232500003, 2009.
- Wang, S., Zheng, J., Fu, F., Yin, S., and Zhong, L.: Development of an emission processing system for the Pearl River Delta Regional air quality modeling using the SMOKE model: Methodology and evaluation, *Atmospheric Environment*, 45, 5079 – 5089, <https://doi.org/https://doi.org/10.1016/j.atmosenv.2011.06.037>, <http://www.sciencedirect.com/science/article/pii/S1352231011006303>, 2011.

Weimer, M., Schröter, J., Eckstein, J., Deetz, K., Neumaier, M., Fischbeck, G., Hu, L., Millet, D., Rieger, D., Vogel, H., Vogel, B., Reddman, T., Kirner, O., Ruhnke, R., and Braesicke, P.: An emission module for ICON-ART 2.0: Implementation and simulations of acetone, *Geoscientific Model Development*, 10, 2471–2494, <https://doi.org/10.5194/gmd-10-2471-2017>, 2017.

- 5 Wong, D. C., Pleim, J., Mathur, R., Binkowski, F., Otte, T., Gilliam, R., Pouliot, G., Xiu, A., Young, J. O., and Kang, D.: WRF-CMAQ two-way coupled system with aerosol feedback: software development and preliminary results, *Geoscientific Model Development*, 5, 299–312, <https://doi.org/10.5194/gmd-5-299-2012>, <https://www.geosci-model-dev.net/5/299/2012/>, 2012.