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# Ocean File: ocean mask and surf zone definition

CMAQ’s land-ocean mask and the fraction of surf zone and open ocean (per grid cell) are read in from a netCDF file denoted as Ocean File. Four Ocean files for the four sea salt emissions cases base, noSurf, zero and full were created and are attached. Below, the general structure of the Ocean File and the procedure applied for creating it are described.

The ocean file contains three variables: MAKS, OPEN and SURF. The variable MASK is the land-coast-ocean mask which defines whether a grid cell is coastline, open ocean or land by taking the values 1, 2 or 0, respectively. SURF and OPEN contain the surf zone and open ocean fractions per grid cell taking values between 0 and 1.

For calculating the surf zone area we imported the coastlines of the Natural Earth large scale data set version 3.1.0 into ArcGIS 10.2.1, added a stripe of 50 m width to the outer side of the coast with the ArcGIS buffer tool and calculated the area within the stripe per grid cell. Overlapping areas of two and more stripes were not counted twice. Open ocean area and land area per grid cell were also calculated by ArcGIS. By looking on Natural Earth coastlines we assumed that coastlines are represented in sufficient resolution.

The resulting ocean file was post processed which is commonly not the case for CMAQ ocean files: First, the surf zone area was limited by a threshold (see below for details). Second, the ocean file was scaled linearly with the salinity (see below for details).

## Limited surf zone

All bights and fjords are included in the ArcGIS calculations. However, in protected bights and fjords there is no surf zone. We arbitrarily defined a maximum effective surf zone shape as plotted in Figure S1. The maximum surf zone fraction in the 24 km grid is calculated in Eq. (S1). The surf zone fraction was capped at this value. The excess area fraction was added to the open ocean area.

Figure S2 (a) shows the surf zone fraction after applying the capping (salinity scaling as described in section S1.2 is already applied). The surf zone fraction that was removed and added to the open ocean is shown in Figure S2 (b). Figure S3 shows the impact of the capping on atmospheric sodium concentrations: cyan cross indicates concentrations without applying the capping. The Waldhof station was exchanged against the Ulborg station that is located directly at the Danish North Sea coast.

|  |  |
| --- | --- |
| Figure S: Maximum effective surf zone. | Figure S: Surf zone fraction per grid cell in %. (a) Surf zone fraction in the base case (capped according to Eq. (S1)). (b) Surf zone fraction that was removed: *[surf zone fraction, no capping] - [surf zone fraction, capping]*. |

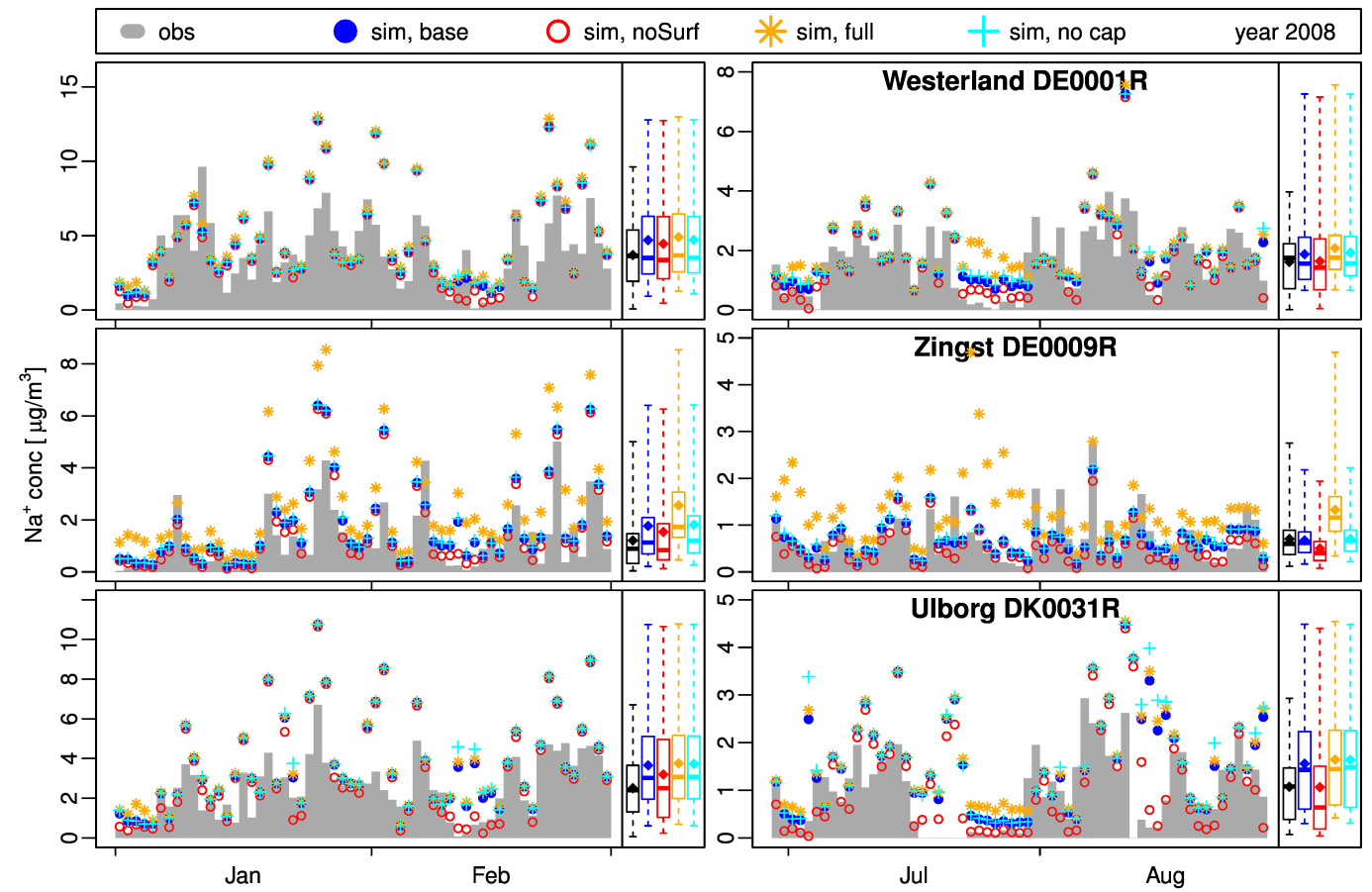


Figure S: Similar to Fig. 5 but with the addition of sodium concentrations without surf zone capping (cross, cyan). Instead of data from the Waldhof station, data from the Danish station Ulborg is shown.

## Salinity Scaling

Martensson et al. (2003) found an effect of salinity on sea salt emissions. Working in the European domain, makes salinity correction of sea salt emissions necessary because the salinity in most parts of the Baltic Sea is below 10‰. In order to reduce sea salt emissions according to local salinity, the values of OPEN and SURF were linearly scaled by the salinity *S*: each value multiplied by *S*/35‰. Martensson et al. (2003) showed, a linear downscaling of the emitted mass, surface and number is not appropriate for the whole size range. However, this linear scaling is the simplest way to add salinity dependence to CMAQ’s sea salt emissions without modifying program code.

The base case Ocean File was created according to this description. The last step was not performed for the full case Ocean File. For the noSurf case Ocean File, SURF was added to OPEN and set to 0 afterwards.

Figure S4 (b) shows the sea surface fraction without being scaled by the salinity. It is 100% above most oceanic regions. Figure S4 (b), in contrast, shows the Ocean file’s sea surface fraction after scaling the actual fraction by *S*/35‰. The red color indicates grid cells with a sea surface fraction above 100% (slightly). This is because the modeled salinity was slightly above 35‰ in the North Sea. The red area in the Atlantic Ocean is an extrapolation artifact.

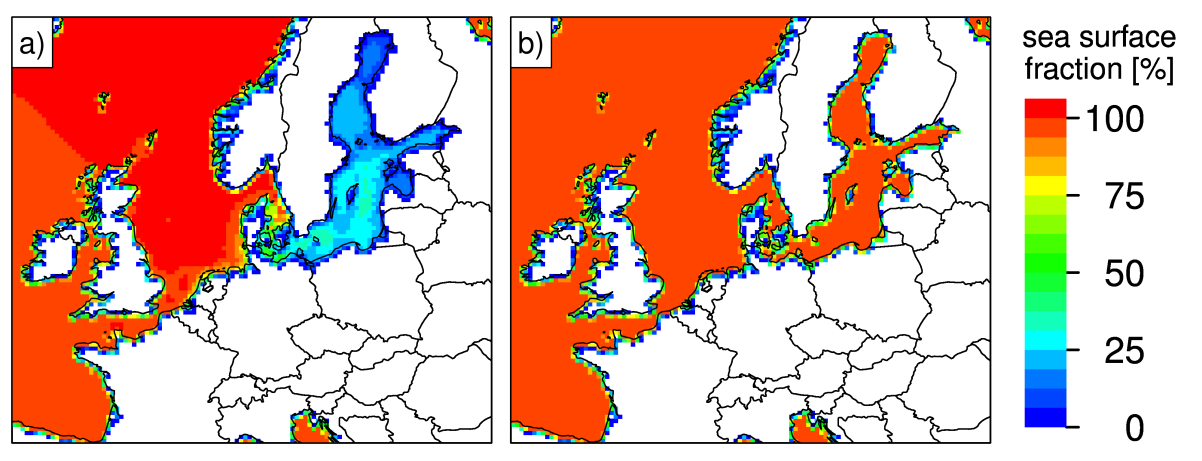


Figure S: Sea surface fraction (OPEN + SURF) in % per grid cell as defined in this study’s Ocean files. (a) Sea surface fraction is scaled by the salinity of the underlying ocean. (b) The original sea surface fraction without salinity scaling.

# Software for Data Evaluation

Data post-processing was performed with Climate Data Operators (cdo) versions 1.5.3 and 1.6.9 and with NetCDF Operators (NCO) versions 4.0.8, 4.0.9, and 4.4.8. Major plotting work and statistical evaluation were performed with R versions 2.15.1 and 3.1.2 using the packages ncdf4, maps, mapdata, cmaqtools and ctmeval. The latter two packages are inh-house developments of our research institute. Figures 1 and 2 were created with Generic Mapping Tools (GMT) version 4.5.2.

# Model Input and Output Data and statistical Evaluation

Those model data which forms the base for plots and statistical evaluations are attached in post-processed format which allows the reproduction of all plots and figures. Data are attached as text (\*.csv) and netCDF (\*.nc) files. Concentration data are located in the subdirectory ‘conc’, sea salt emission data in the subdirectory ‘ssemis’, and nitrogen deposition data in the subdirectory ‘ndep’.

Table S: List of attached files containing model output data.

|  |  |  |  |
| --- | --- | --- | --- |
| **Type** | **Comment** | **Files** | **Corresp. Fig.** |
| Sea Salt Emissions | averaged in time; resolved in space; one season (summer | winter) and one case (base | noSurf) per file; | ssemis.area.timemean.\*.nc  (four files) 1 | 3 (sum of ANAJ, ANAK, ACLJ, ACLK, ASO4J and ASO4K plotted) |
| Sea Salt Emissions | hourly resolved in time; one location (A | B | C), one season (summer | winter) and one case (base | noSurf) per file; | ssemis.timeseries.\*.csv  (12 files) | 4 (MASST plotted) |
| Concen-trations | hourly resolved in time; data on each station (see Table in section D); one species (Na+ | xSO4 | sNH4 | sNO3), one season (summer | winter) and one case (base | noSurf | full | zero) per file | conc.timeseries.\*.csv  (32 files) | 5, 6, 7, and 8 |
| Nitrogen Wet Deposition | Nitrogen wet deposition averaged over the time intervals for which measurement data are available; one case (base | noSurf | full | zero) and one station per file | wetdep.timeseries.\*.csv  (56 files) | 10 |
| Nitrogen Deposition | averaged in time; resolved in spaces; one season (summer | winter) and one case (base | noSurf | zero | full) per file | ndep.area.timemean.\*.nc  (8 files) 1 | 9 |

1 J and K in variable names indicate accumulation and coarse mode particle mass/number, respectively. T indicates total mass/number (J + K). ANA, ACL and ASO4 denote Na+, Cl- and SO42- emissions, respectively.

Open ocean and surf zone fraction per grid cell are needed for calculating sea salt emissions in CMAQ (see Table S2). Additionally, these data are needed for the simulation result evaluation. The files are located in the subdirectory ‘cmaq’.

Table S: Input files for CMAQ. Files are also needed for the data evaluation.

|  |  |  |  |
| --- | --- | --- | --- |
| **Type** | **Comment** | **Files** | **Corresp. Fig.** |
| Sea Surface Fraction | Ocean file needed for sea salt emissions in CMAQ; contains OPEN (open ocean fraction), SURF (surf zone fraction), and MASK (0 = land; 1 = coast; 2 = open ocean) | \*sf050m\*ubound\_sal.nc (base)  \*sf000m\*ubound.nc (noSurf)  \*noSalt\*.nc (zero)  \*sf050m\*ubound.nc (full)  \*sf050m\*sal.nc (no surf zone fraction capping) | S4 and S5 |

Data on the statistical evaluation are in the file ‘statistical.evaluation.conc.csv’ in the directory ‘conc’ and in ‘statistical.evaluation.wetdep.csv’ in ‘n\_wetdep’. They contain

* n (number of considered values),
* RAE (residual absolute error),
* MNB (mean normalized bias),
* R (Spearman’s correlation coefficient),
* MEAN.sim (mean of considered model values),
* MEAN.obs (mean of considered EMEP values),
* MEDIAN.sim (median of considered model values), and
* MEDIAN.obs (median of considered EMEP values).

# EMEP data

EMEP data for the comparison can be obtained from the EBAS database at <http://ebas.nilu.no>. Data for the year 2008 for the following stations were obtained for the evaluation of model data.

Table s: EMEP stations at which model and measurement data were compared statistically.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Station ID** | **Station Name** | **Data** | **Lon** | **Lat** | **Height [m]** | **Location** |
| DE0001R | Westerland | Na+, (NO3-,) sNO3, sNH4 | 8.31 | 54.93 | 12 | Coast |
| DE0002R | Waldhof | Na+, (NO3-,) sNO3, sNH4 | 10.76 | 52.80 | 74 | Inland |
| DE0007R | Neuglobsow | Na+, (NO3-,) sNO3, sNH4 | 13.03 | 53.17 | 62 | Inland |
| DE0009R | Zingst | Na+, (NO3-,) sNO3, sNH4 | 12.73 | 54.43 | 1 | Coast |
| DE0044R | Melpitz | Na+, NO3- | 12.93 | 51.53 | 86 | Inland |
| DK0003R | Tange | Na+, sNO3, sNH4 | 9.60 | 56.35 | 13 | Inland |
| DK0005R | Keldsnor | Na+, sNO3, sNH4 | 10.73 | 54.73 | 10 | Coast |
| DK0008R | Anholt | Na+, sNO3, sNH4 | 11.52 | 56.72 | 40 | Coast |
| DK0031R | Ulborg | Na+, sNO3, sNH4 | 8.43 | 56.28 | 10 | Coast |
| FI0009R | Utö | Na+, sNO3, sNH4 | 21.38 | 59.78 | 7 | Coast |
| FI0017R | Virolahti II | Na+, sNO3, sNH4 | 27.69 | 60.53 | 4 | Coast |
| NO0001R | Birkenes | Na+, (NO3-,) sNO3, sNH4 | 8.25 | 58.38 | 190 | Mixed |
| NO0056R | Hurdal | Na+, (NO3-,) sNO3, sNH4 | 11.08 | 60.37 | 300 | Inland |
| PL0002R | Jarczew | (NO3-,) sNO3, sNH4 | 21.98 | 51.82 | 180 | Inland |
| PL0004R | Leba | (NO3-,) sNO3, sNH4 | 17.53 | 54.75 | 2 | Coast |
| SE0014R | Råö | sNO3, sNH4 | 11.91 | 57.39 | 5 | Coast |
|  |  |  |  |  |  |  |

# Nitrogen Deposition

The nitrogen deposition per grid cell was multiplied by the sea surface fraction per grid cell for calculating the nitrogen deposition into the sea. Thus, in a coastal grid cell with 40% sea surface and 60% land, only 40% of the nitrogen deposition is considered. Figure S5 shows the sea surface fraction and the regions that are considered as North and Baltic Sea. The latter information is necessary to create Table 6.

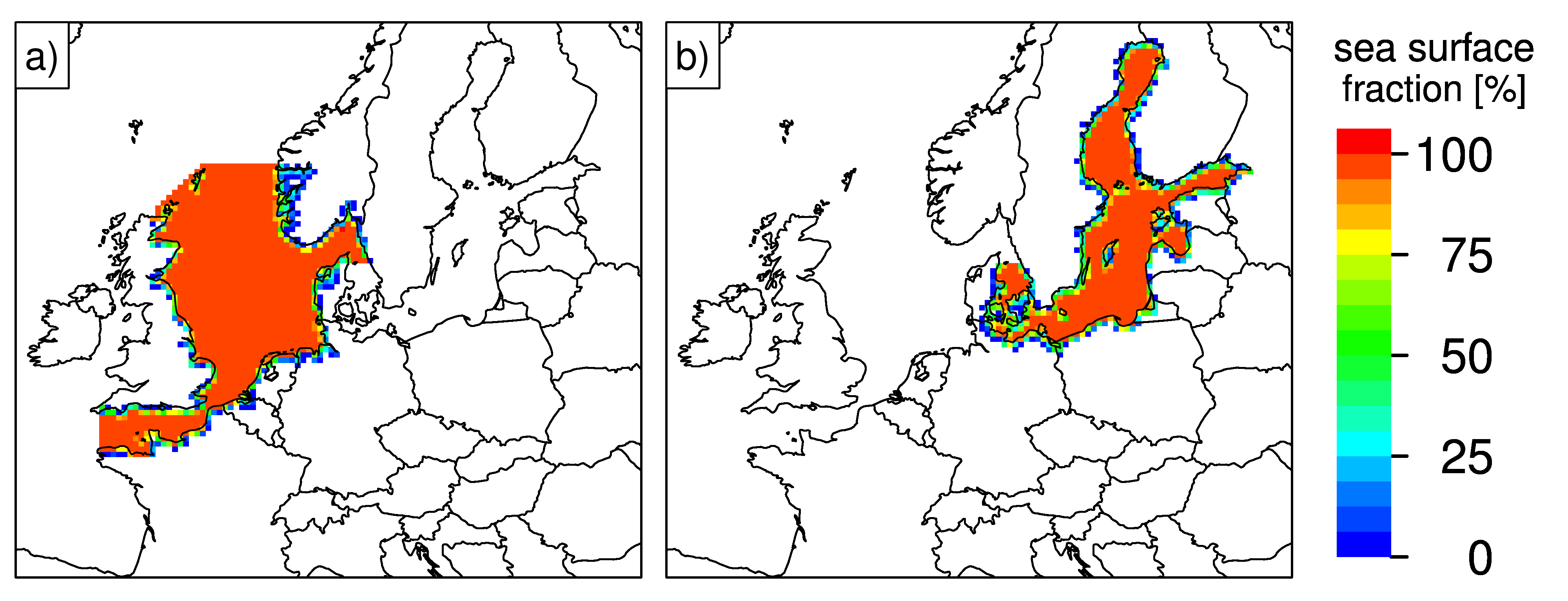


Figure S: Sea surface fraction of North (a) and Baltic Sea (b) that is considered for calculating the nitrogen deposition into both seas.