

A 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: MASK, 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 1. The maximum surf zone coverage in the 24 km grid is calculated in Eq. (A1). The excess area fraction was added to the open ocean area.

$$\text{SURF}_{mx} = \frac{(\sqrt{5} * 50 \text{ m} * 24 \text{ km})}{(24 \text{ km})^2} = \frac{\sqrt{5} * 50 \text{ m}}{24 \text{ km}} = 0.004658 \approx 0,47\% \quad (\text{A1})$$

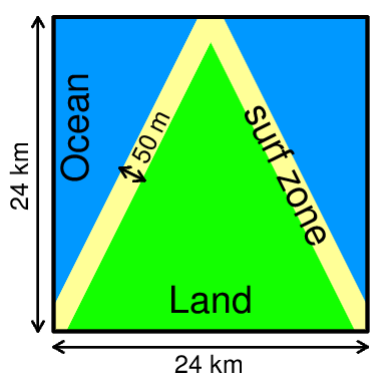


Figure 1: Maximum effective surf zone.

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 $S/0.035$. 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.

B 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 ncd4, maps, mapdata, cmaqtools and ctmeval. The latter two packages are in-house developments of our research institute. Figures 1 and 2 were created with Generic Mapping Tools (GMT) version 4.5.2.

C Available Model Data

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.

Table 1: List of attached files containing model 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)	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)
Concentrations	hourly resolved in time; data on each station (see Table in section D); one species (Na ⁺ xSO ₄ sNH ₄ sNO ₃), one season (summer winter) and one case (base noSurf full zero) per file	conc.timeseries.*.csv (32 files)	5, 6, 7 and 8

J and K in variable names and headings 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. Day in table headings abbreviates “day of year”.

D 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 2: EMEP stations at which model and measurement data were compared statistically.

Station ID	Station Name	Nation	Longitude	Latitude	Height
DE0001R	Westerland	DE	8,31	54,93	12
DE0002R	Waldhof	DE	10,76	52,80	74
DE0003R	Schauinsland	DE	7,91	47,91	1205
DE0007R	Neuglobsow	DE	13,03	53,17	62

DE0009R	Zingst	DE	12,73	54,43	1
DK0003R	Tange	DK	9,60	56,35	13
DK0005R	Keldsnor	DK	10,73	54,73	10
DK0008R	Anholt	DK	11,52	56,72	40
DK0031R	Ulborg	DK	8,43	56,28	10
NO0001R	Birkenes	NO	8,25	58,38	190
NO0056R	Hurdal	NO	11,08	60,37	300
PL0002R	Jarczew	PL	21,98	51,82	180
PL0003R	Snieszka	PL	15,73	50,73	1603
PL0004R	Leba	PL	17,53	54,75	2
SE0014R	Råö	SE	11,91	57,39	5

E Station comparison data

Data on the statistical evaluation are attached in the file statistical.evaluation.csv. It contains

- n (number of considered values),
- rae (residual absolute error),
- mnb (mean normalized bias),
- cor (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)

for each of the considered

- stations (15 stations listed in section D),
- species (Na^+ , xSO_4 , sNH_4 and sNO_3),
- seasons (winter and summer) and
- sea salt emission cases (base, noSurf, zero and full).