

# The EMEP/MSC-W Model - User's Guide

February 2014

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# Chapter 1

## Welcome to EMEP

This guide gives a brief documentation of the EMEP/MSC-W model version rv4.4. It is intended primarily as a guide on how to run the model, and to help users wishing to understand or change the model in terms of domains, outputs, chemistry, etc.

The main documentation for the EMEP/MSC-W model is an article published in Atmospheric Chemistry and Physics 2012. This article will be referred to as Simpson et al. (2012) in this manual.

- Simpson, D., Benedictow, A., Berge, H., Bergström, R., Emberson, L.D., Fagerli, H., Flechard, C.R., Hayman, G.D., Gauss, M., Jonson, J.E., Jenkin, M.W., Nyíri, A, Richter, C., Semeena, V.S, Tsyro, S., Tuovinen, J.-P., Valdebenito, Á., and Wind, P., The EMEP MSC-W chemical transport model technical description. Atmospheric Chemistry and Physics, 12, 7825-7865, <http://www.atmos-chem-phys.net/12/7825/2012/acp-12-7825-2012.html>

The model source code is available from the EMEP/MSC-W Open Source website:  
[https://wiki.met.no/emep/page1/emepmscw\\_opensource](https://wiki.met.no/emep/page1/emepmscw_opensource)

## 1.1 Licenses and Caveats

The EMEP code is provided under the GNU General Public License version 3 (<http://fsf.org> and/or <http://www.gnu.org/copyleft/gpl.html>).

Each code module is prefaced with something like:

```
! <EXAMPLE_CODE.f90 - A component of the EMEP MSC-W Unified Eulerian
!     Chemical transport Model>
!*****!
!*
!* Copyright (C) 2007-2012 met.no
!*
!* Contact information:
!* Norwegian Meteorological Institute
!* Box 43 Blindern
!* 0313 OSLO
!* NORWAY
!* email: emep.mscw@met.no
!*
!* This program is free software: you can redistribute it and/or modify
!* it under the terms of the GNU General Public License as published by
!* the Free Software Foundation, either version 3 of the License, or
!* (at your option) any later version.
!*
!* This program is distributed in the hope that it will be useful,
!* but WITHOUT ANY WARRANTY; without even the implied warranty of
!* MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
!* GNU General Public License for more details.
!*
!* You should have received a copy of the GNU General Public License
!* along with this program. If not, see <http://www.gnu.org/licenses/>.
!*****!
```

And a copy of the license file, **gpl.txt**, is provided with the model code source files.

It is important to note that the code is provided “as it is”, and EMEP/MSW-W has very limited resources with which to support code-usage. To help users an **EMEP Forum** is available from the EMEP/MSW-W Open Source website in section “Users”: “EMEP Forum”. Support to the user community will develop here with your contribution. Please let us know what your needs for information are (e-mail: [emep.mscw@met.no](mailto:emep.mscw@met.no)).

## 1.2 Computer Information

To compile the EMEP/MSC-W model you need:

**Fortran 95 compiler**

**NetCDF Library (>4.1.3)**

**MPI Library (>1.0)**

It is necessary to compile with double precision reals (8 bytes reals). The program has been used on computers ranging from a Linux laptop to supercomputers (Itanium2 cluster, Intel Xeon cluster, Cray XT4, IBM power5+). It is compatible with all compilers tested so far: Intel, PGI, gfortran, XL fortran. A Makefile is included, the path to netcdf (INCL and LLIB) have to be adapted to your machine, and the fortran compiler (F90) and flags (F90FLAGS) to the compiler you are using.

The code has been tested with 1 to 1024 CPUs, and scales well (for large grids). If only one CPU is used 1-2 GB memory is required. If more than one, for example 64 CPUs are used, 200 MB of memory per CPU is enough (in the case of a 132 X 159 grid size). For runs on more than 32 CPUs, a fast interconnect is recommended (infiniband for example), for smaller runs, gigabit ethernet is sufficient. It takes  $\sim 5$  hrs on 64\*Xeon X5355 (2.66GHz) for 1 year simulation.

When downloading input data in order to do a “base run” please make sure that there are 35 Gb disc space available, especially due to large meteorology input files. The model can be run for shorter periods, users can download meteorology for only the period they are interested in, plus one day.

## 1.3 Getting Started

It is recommended to read all the chapters of this EMEP/MSC-W model User Guide before you start downloading anything from the EMEP/MSC-W Open Source website.

Please register as an EMEP User on the **EMEP Forum** (EMEP/MSC-W Open Source website under “Users” section: “EMEP Forum”) before you start downloading the EMEP/MSC-W model code and/or input data. This will give you access to further communication with the developing team and to the section on “Questions and Answers”.

This is what you need to do before you can do a “base run” with the EMEP/MSC-W model:

- Register as an EMEP User
- Read the EMEP/MSC-W model User Guide
- Download input data (description in Chapter 2 and data available from the EMEP/MSC-W Open Source website under “Download” section: “Input Data”)
- Download the EMEP/MSC-W model source code (description in section 1.4 and the files are available from the EMEP/MSC-W Open Source website under “Download” section: “Model Code”)
- Follow the instructions for ‘Submitting a Run’ description in Chapter 4.

- Download some model results for comparison, description in Chapter 3 and the files are available from the EMEP/MSC-W Open Source website under “Download” section: “Model Results”.

## 1.4 Model code

The EMEP/MSC-W model code version rv.4\_4 are archived as a tar file. The tar file is called “EMEP\_MSC-W\_model.rv4\_4.OpenSource.tar.gz” and is downloadable from the EMEP/MSC-W Open Source website.

Once this file is untarred all model files needed for a model run will be found under the directory

**EMEP\_MSC-W\_model.rv4\_4.OpenSource/code/** where the model source code, makefiles, and a copy of the license file are stored. An overview is given in Table 1.1

Table 1.1: Contents of “EMEP\_MSC-W\_model.rv4\_4.OpenSource.tar” file

| Type                        | Filename                               |
|-----------------------------|--|
| <b>Model code directory</b> | EMEP_MSC-W_model.rv4_4.OpenSource/code |
| modules files               | *.f90                                  |
| include files               | *.inc                                  |
| namelist                    | config_emep.nml                        |
| makefiles                   | Makefile and Makefile.SRCS             |
| dependency file             | dependencies                           |
| a copy of the license       | gpl.txt                                |

In addition there is a run script called “modrun.sh”, which will be placed in the **EMEP\_MSC-W\_model.rv4\_4.OpenSource/** directory. The run script, “modrun.sh”, can easily be modified to work on your computer system. This script is described in detail in Chapter 4.

## 1.5 Model grid

The current EMEP model version, and the provided gridded input data, have a horizontal resolution of  $50 \times 50$  km<sup>2</sup> (at 60°N) and are defined on a polar stereographic projection with 20 sigma levels vertically. The model is very flexible with regard to the horizontal resolution, in that it readily makes use of meteorological data provided with the model. The vertical resolution is currently still restricted to the fixed 20 layer system. The physical description is given in detail in Chapter 2 of the EMEP Status Report 1/2003 Part I (Simpson *et al.*, 2003).

In 2008 the official EMEP domain was extended eastwards in order to include the EECCA countries in the EMEP model grid, see Figure 1.1. To distinguish the new grid from the old EMEP grid, the new grid is called EECCA in this text and in the config\_emep.nml.

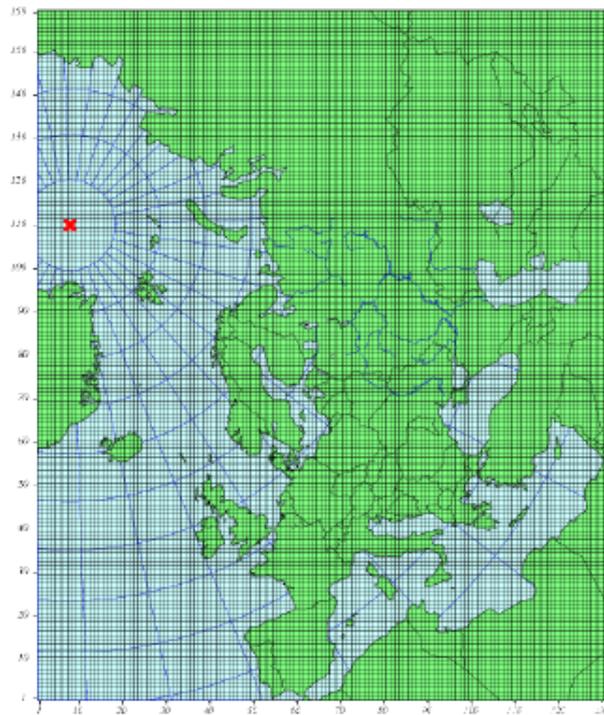


Figure 1.1: The extended EMEP grid covering EECCA area with  $132 \times 159$  gridpoints on  $50 \times 50 \text{ km}^2$  resolution defined on a polarstereographic projection.

# Chapter 2

## Input files

This chapter provides an overview on the necessary input files to run the EMEP/MSC-W model. A complete set of input files is provided in the EMEP/MSC-W Open Source web page to allow model runs for the meteorological year 2010 and 2011.

The input files are zipped in 13 different files. There are 12 zipped files for the meteorology, one for each month, called meteo2010MM.tar.bz2 and meteo2011MM.tar.bz2 (where MM is the month). The last file for December also include a met file for January 1<sup>st</sup> 2011 and 2012 respectively. The last zipped input file (called other\_input\_files.tar.bz2) contains all other input files needed for running the EMEP/MSC-W model, except the aircraft emissions, AircraftEmis\_FL.nc, and the forest fire emissions, FINN\_ForestFireEmis\_2010.nc. See sections 2.1.8 and 2.1.10 for details about these emissions data.

After unzipping all the meteo-tar files, the meteorology are placed under a catalogue called **EMEP\_Unified\_model.OpenSource2013/**. The met/ catalogue should be moved over to current version of model, for rv4\_4: **EMEP\_MSC-W\_model.rv4\_4.OpenSource**. So now there will be two directories under **EMEP\_MSC-W\_model.rv4\_4.OpenSource**. All meteorology are placed under /met, and the rest of the input files under /input. All files, both meteorological and the other input files, are described in this chapter.

**IMPORTANT:** The input data available in the EMEP/MSC-W Open Source Web site should be appropriately acknowledged when used for model runs. If nothing else is specified according to references further in this chapter, please acknowledge EMEP/MSC-W in any use of these data.

Table 2.1: List of input data files. Note: YYYY: year, MM: month, DD: day, SS: seasons, POLL: pollutant type (NH<sub>3</sub>, CO, NO<sub>x</sub>, SO<sub>x</sub>, NMVOC, PM<sub>2.5</sub> and PM<sub>co</sub>).

| <b>Data</b>                          | <b>Name</b>                            | <b>Format</b> |
|--------------------------------------|--|---------------|
| <b>Meteorology data</b>              | met/                                   |               |
| Meteorology                          | meteoYYYYMMDD.nc (365+1 files)         | netCDF        |
| <b>Other Input files</b>             | input/                                 |               |
| Global Ozone                         | GLOBAL_O3.nc                           | netCDF        |
| BVOC emissions                       | EMEP_EuroBVOC.nc                       | netCDF        |
| Landuse                              | LanduseGLC.nc and Landuse_PS_5km_LC.nc | netCDF        |
| Degree-day factor                    | DegreeDayFactors.nc                    | netCDF        |
| N depositions                        | annualNdep.nc                          | netCDF        |
| Road dust                            | RoadMap.nc and AVG_SMI_2005_2010.nc    | netCDF†       |
| Aircraft emissions                   | AircraftEmis_FL.nc                     | netCDF†       |
| Surface Pressure                     | SurfacePressure.nc                     | netCDF†       |
| Forest Fire                          | FINN_ForestFireEmis_YYYY.nc            | netCDF†       |
| Natural SO <sub>2</sub>              | natso2MM.dat (12 files)                | ASCII         |
| Volcanoes                            | VolcanoesLL.dat                        | ASCII*        |
|                                      | eruptions.csv volcanoes.csv            | ASCII         |
| Emissions                            | emislist.POLL (7 files)                | ASCII         |
| Time factors for monthly emissions   | MonthlyFac.POLL (7 files)              | ASCII         |
| Time factors for daily emissions     | DailyFac.POLL (7 files)                | ASCII         |
| Time factors for hourly emissions    | HOURLY-FACS                            | ASCII*        |
| Emission heights                     | EmisHeights.txt                        | ASCII*        |
| Landuse definitions                  | Inputs_LandDefs.csv                    | ASCII*        |
| Stomatal conductance                 | Inputs_DO3SE.csv                       | ASCII*        |
| Lightning emissions                  | lightningMM.dat (12 files)             | ASCII*        |
| Emissions speciation                 | emissplit.defaults.POLL                | ASCII*        |
|                                      | emissplit.specials.POLL                | ASCII*,†      |
| Photo-dissociation rates             | jclearSS.dat (4 files)                 | ASCII         |
|                                      | jcl1kmSS.dat (4 files) + jcl1.jun      | ASCII         |
|                                      | jcl3kmSS.dat (4 files) + jcl3.jun      | ASCII         |
| Dust files                           | sand_frac.dat clay_frac.dat            | ASCII†        |
|                                      | DUST_f.MM DUST_c.MM                    | ASCII†        |
|                                      | SoilTypes_IFS.nc                       | netCDF†       |
| Sites locations for surface output   | sites.dat                              | ASCII*        |
| Sondes locations for vertical output | sondes.dat                             | ASCII*        |
| Emission factors for scenario runs   | femis.dat                              | ASCII         |

Notes: † - optional (in most cases); \* means ASCII files with header.

## 2.1 NetCDF files

### 2.1.1 Meteorology

The daily meteorological input data (“meteoYYYYMMDD.nc”, where YYYY is year, MM is month and DD is day) used for the EMEP/MSC-W Model are based on forecast experiment runs with the Integrated Forecast System (IFS), a global operational forecasting model from the European Centre for Medium-Range Weather Forecasts (ECMWF).

The IFS forecasts has been run by MSC-W as independent experiments on the HPCs at ECMWF with special requests on some output parameters. The meteorological fields are retrieved on a  $0.2^\circ \times 0.2^\circ$  rotated spherical grid and interpolated to  $50 \times 50 \text{ km}^2$  polar-stereographic grid projection. Vertically, the fields on 60 eta levels from the IFS model are interpolated onto the 20 EMEP sigma levels. The version of the IFS model used for preparing these fields, Cycle 36r1, is documented in <http://www.ecmwf.int/research/ifsdocs/index.html>. Meteorological fields currently used for EMEP/MSC-W Model runs are given in Table 2.2. Some verification and description of these meteorological fields are given in Chapter 7 of the EMEP Status Report 1/2010.

**Acknowledgement:** ECMWF, met.no

Table 2.2: Input meteorological data used in the EMEP/MSC-W Model

| Parameter                          | Unit                           | Description                         |
|------------------------------------|--------------------------------|-------------------------------------|
| 3D fields - for 20 $\sigma$ levels |                                |                                     |
| $u, v$                             | m/s                            | Horizontal wind velocity components |
| $q$                                | kg/kg                          | Specific humidity                   |
| $\theta$                           | K                              | Potential temperature               |
| $CW$                               | kg/kg                          | Cloud water                         |
| $CL$                               | %                              | 3D Cloud cover                      |
| $cnvuf$                            | kg/sm <sup>2</sup>             | Convective updraft flux             |
| $cnvdf$                            | kg/sm <sup>2</sup>             | Convective downdraft flux           |
| $PR$                               | mm                             | Precipitation                       |
| 2D fields - for Surface            |                                |                                     |
| $PS$                               | hPa                            | Surface pressure                    |
| $T2$                               | K                              | Temperature at 2m height            |
| $Rh2$                              | %                              | Relative humidity at 2m height      |
| $SH$                               | W/m <sup>2</sup>               | Surface flux of sensible heat       |
| $LH$                               | W/m <sup>2</sup>               | Surface flux of latent heat         |
| $\tau$                             | N/m <sup>2</sup>               | Surface stress                      |
| $SST$                              | K                              | Sea surface temperature             |
| $SWC$                              | m <sup>3</sup> /m <sup>3</sup> | Soil water content                  |
| $lspr$                             | m                              | Large scale precipitation           |
| $cpr$                              | m                              | Convective precipitation            |
| $sdepth$                           | m                              | Snow depth                          |
| $ice$                              | %                              | Fraction of ice                     |
| $SMI1$                             |                                | Soil moisture index level 1         |
| $SMI3$                             |                                | Soil moisture index level 3         |
| $u10/v10$                          | m/s                            | wind at 10 m height                 |

### 2.1.2 Global Ozone

Initial concentration of ozone are required in order to initialize the model runs. Boundary conditions along the sides of the model domain and at the top of the domain are then required as the model is running.

The GLOBAL\_O3.nc file contains monthly averaged fields in netCDF format. The initial and background concentrations are based on the Logan (1998) climatology. The Logan climatology is scaled by Unimod according to the Mace Head measurements as described in Simpson *et al.* (2003). For a number of other species, background/initial conditions are set within the model using functions based on observations (Simpson *et al.*, 2003 and Fagerli *et al.*, 2004).

### 2.1.3 BVOC emissions

Biogenic emissions of isoprene and monoterpene are calculated in the model as a function of temperature and solar radiation, using the landuse datasets. The light and temperature dependencies are similar to those used in the original open source model, see Chapter 4.2 of the EMEP Status Report 1/2003 Part I (Simpson *et al.*, 2003).

Biogenic VOC emission potentials (i.e. rates at 30°C and full sunlight) are included for four different forest types in the netCDF file EMEP\_EuroBVOC.nc. These emission potentials have unit  $\mu\text{g}/\text{m}^2/\text{h}$ , and refer to emissions per area of the appropriate forest category. In addition, default emission potentials are given for other land-cover categories in the file Inputs\_LandDefs.csv. The underlying emission potentials, land-cover data bases, and model coding have however changed substantially since model version v.2011-06. The new approach is documented in Simpson *et al.*, 2012.

### 2.1.4 Landuse

Landuse data are required for modeling boundary layer processes (i.e. dry deposition, turbulent diffusion). The EMEP/MSC-W model can accept landuse data from any data set covering the whole of the domain, providing reasonable resolution of the vegetation categories. Gridded data sets providing these landuse categories across the EMEP domain have been created based on the data from the Stockholm Environment Institute at York (SEI-Y) and from the Coordinating Center for Effects (CCE). 16 basic landuse classes have been identified for use in the deposition module in the model, and three additional “fake” landuse classes are used for providing results for integrated assessment modeling and effects work.

There are two netcdf files included, one file “Landuse\_PS\_5km\_LC.nc” on 5 km resolution over the EMEP domain, and a global “LanduseGLC.nc”. The different landuse types are described in Simpson *et al.* (2012).

### 2.1.5 Degree-day factor

Domestic combustion which contribute to a large part of SNAP-2, varies on the daily mean temperature. The variation is based on the heating degree-day concept. These degree days are pre-calculated for each day and stored in the file DegreeDayFactors.nc. See Simpson *et al.* (2012) section 6.1.2.

### 2.1.6 NO<sub>x</sub> depositions

Areas with high NO deposition loads have greater soil-NO emissions. To include this in the model, a netcdf file where pre-calculated N-depositions are included. The file made by the results from the EMEP/MSC-W model runs over a 5-year period.

### 2.1.7 Road Dust

Road traffic produces dust. These emissions are handled in the EMEP/MSC-W model in the **Emissions\_ml.f90** module. To include road dust, set `USE_ROADDUST = .true.` in “`config_emep.nml`”. There are two files included in input data, `RoadMap.nc` and `AVG_SMI_2005-2010.nc`. `RoadMap.nc` include gridded roads and PM emissions over Europe, `AVG_SMI_2005-2010.nc` are global.

### 2.1.8 Aircraft emissions

In the EMEP/MSC-W model aircraft emissions are 'OFF' by default. They can be switched 'ON' by setting `USE_AIRCRAFT_EMIS = .true.` in “`config_emep.nml`” and download the data from <http://www.pa.op.dlr.de/quantify>. The EMEP model uses data provided by the EU-Framework Programme 6 Integrated Project QUANTIFY (<http://www.pa.op.dlr.de/quantify>). However, before using these data a protocol has to be signed, which is why the data file can not be provided directly on the EMEP/MSC-W Open Source website. If you want to use aircraft emissions go to <http://www.pa.op.dlr.de/quantify>, click on 'QUANTIFY emission inventories and scenarios', and then click on 'Register'. That page will provide information about the registration process and the protocol that has to be signed. Once you are registered, click 'Login' and provide user name and password. On the new page, search for 'Emissions for EMEP', which links directly to the Readme file and the emission data file in netCDF format. Download the emission data file and place it in the input folder.

### 2.1.9 Surface Pressure

If `USE_AIRCRAFT_EMIS = .true.` in **ModelConstants\_ml.f90**, then in addition to the Aircraft Emission file, there will be need for a `SurfacePressure.nc` file, which is already in the /input folder. The netCDF file consists of surface pressure fields for each of the months in 2008 called `surface_pressure`, and one field for the whole year called `surface_pressure_year`. All fields are given in Pa.

### 2.1.10 Forest Fire

As of model version rv3.9 (November 2011), daily emissions from forest and vegetation fires are taken from the Fire INventory from NCAR version 1.0 (FINNv1, Wiedinmyer et al. 2011). Data are available from 2005, with daily resolution, on a fine 1 km1 km grid. We store these data on a slightly coarser grid (0.2°0.2°) globally for access by the EMEP/MSC-W model. To include forest fire emissions set `USE_FOREST_FIRES = .true.` in “`config_emep.nml`” and download the 2010 GEOS-chem daily data <http://bai.acd.ucar.edu/Data/fire/>. The data needs to be stored with units mole/day in a netCDF file called `FINN_ForestFireEmis_2010.nc` compatible with the **ForestFire\_ml.f90** module.

## 2.2 ASCII files

### 2.2.1 Natural $SO_2$

Natural  $SO_2$  emissions (dimethylsulfide (DMS) from sea) are provided as monthly gridded files. The values are given at the surface in  $\mu\text{g}/\text{m}^2$  for each grid cell in the domain.

### 2.2.2 Volcanoes

Emissions from volcanoes are included for Italy, based upon the officially submitted data. To consider the volcanic emissions, we need to feed the location and height of volcanoes into the model.

The input file “VolcanoesLL.dat” in **ASCII** format contains the input data for the two active volcanoes Enta and Stromboli. The two first columns gives their latitudes and longitudes, their height as sigma level in column 3 and their emission in ktons per year in column 4.

To include the 2010 volcanic eruptions of Eyjafjallajökull on Iceland additional files are included. Since volcano only had eruptions on some days, two files are included. The first “volcanoes.cvs” gives the name of the volcano, and “eruption.cvs” gives date and amount of ash and  $SO_2$  emissions. This is further described in Mastin *et al.*, 2009a and Mastin *et al.*, 2009b.

### 2.2.3 Gridded Emissions

The emission input for the EMEP/MSC-W model consists of gridded annual national emissions based on emission data reported every year to EMEP/MSC-W (until 2005) and to CEIP (from 2006) by each participating country. More details about the emission input with references can be found in Chapter 4 of the EMEP Status Report 1/2003 Part I (Simpson *et al.*, 2003).

The 7 gridded emission input files “emislist.poll” are available in **ASCII** format for the following compounds: CO,  $NH_3$ ,  $NO_x$ ,  $PM_{2.5}$ ,  $PM_{co}$ ,  $SO_x$  and VOC.

The gridded emission files contain 16 columns where the first column represents the country code ([http://www.emep.int/grid/country\\_numbers.txt](http://www.emep.int/grid/country_numbers.txt)), the second and the third columns are the ‘i’ and ‘j’ indices of the EMEP grid, the fourth and fifth columns are the total emissions from low and high sources, and the last 11 columns contain emissions from 10 anthropogenic SNAP sectors ([http://reports.eea.eu.int/technical\\_report\\_2001\\_3/en](http://reports.eea.eu.int/technical_report_2001_3/en)) and 1 source-sector called “Other sources and sinks”, which include natural and biogenic emission sources. The data are given with the unit: *Mg*.

**Acknowledgement:** EMEP

### 2.2.4 Time factors for emissions

Monthly and daily time factors for emission of the 7 compounds (CO,  $NH_3$ ,  $NO_x$ ,  $PM_{2.5}$ ,  $PM_{co}$ ,  $SO_x$  and VOC). There is one file available per compound in **ASCII** format.

The first two columns in the files represent the country code ([http://www.emep.int/grid/country\\_numbers.txt](http://www.emep.int/grid/country_numbers.txt)), the second column represents the sector (<http://webdab.emep.int/sectors.html>). In the monthly files, the 12 consecutive columns

represent the time factors corresponding to the months of the year. In the daily files there are 7 consecutive columns representing the time factor for each day of the week.

The file HOURLY-FACS includes factors for each of the eleven SNAP sectors for every hour (the columns) for each day of the week, see Simpson et al. (2012) section 6.1.2

### 2.2.5 Emission heights

A vertical distribution for the eleven SNAP sectors are given in the file EmisHeights.txt. The file has seven vertical levels, over the columns and the SNAP sectors given in the first row. Read more in Simpson et al. (2012) section 6.1.1.

### 2.2.6 Emission factor for scenario runs

Scenario run in the case of the EMEP/MSC-W model means a run to test the impact of one or more pollutants from a particular country.

Emission factors are applied to specified countries and emission sectors and can be set by changing the ASCII file “femis.dat”. This file can be changed by the users according to their needs.

The file contains several columns (the number is flexible). The first column represents the country code ([http://www.emep.int/grid/country\\_numbers.txt](http://www.emep.int/grid/country_numbers.txt)), the second represents the sector ([http://reports.eea.eu.int/technical\\_report\\_2001\\_3/en](http://reports.eea.eu.int/technical_report_2001_3/en)) where ‘0’ means all sectors, and then in the remaining columns one can specify which emissions to reduce. Here 1.0 means no reduction of the given pollutant (sox/nox/voc/nh3/co/pm25/pmco) from sectors of specified country. The number following the first text (“Name”) in line 1 (number 5 in the downloaded file) gives the number of pollutants treated in the file.

### 2.2.7 Chemical speciation of emissions

Many of the emission files give emissions of a group of compounds, e.g. NO<sub>x</sub> includes NO+NO<sub>2</sub>, and VOC can include many compounds. The information needed to retrieve emissions of individual compounds from these the gridded files is given in files labelled *emissplit.defaults.poll* or *emissplit.specials.poll*, where *poll* can be nox, voc, etc.

The defaults file give the emission split for each SNAP sector (one per row, with second index being the SNAP sector), which is applied to all countries by default. For VOC this split was derived from the UK inventory of Passant (2002), as part of the chemical comparison project of Hayman *et al.* (2011).

The specials files are in general optional, and can be used to specify speciation for particular countries or SNAP sectors. The 1<sup>st</sup> column specifies the country code of interest, the second the SNAP sector.

If forest fires are used, then the file *emissplit.specials.voc* is required (not optional), and the country-code 101 used to specify the VOC speciation of forest fires in this file.

## 2.2.8 Lightning emissions

Emissions of  $\text{NO}_x$  from lightning are included in the model as monthly averages on a T21 ( $5.65^\circ \times 5.65^\circ$ ) resolution (Køhler *et al.*, 1995). The lightning emissions are defined on a  $64 \times 32$  grid with 17 vertical levels, with global coverage, and are provided as 12 ASCII files “lightningMM.dat”.

## 2.2.9 Landuse definitions

For the vegetative landuse categories where stomatal modeling is undertaken, the start and end of the growing season (SGS, EGS, in days) must be specified. The calculation of SGS and EGS with respect to latitude is done in the module **LandDefs\_ml.f90**. The parameters needed to specify the development of the leaf area index (LAI) within the growing season are given in the ASCII file “Inputs\_LandDefs.csv”. For more information, see chapter 5 of the EMEP Status Report 1/2003 Part I (Simpson *et al.*, 2003).

The file, designed to be opened with excel or gnumeric, contains a header briefly explaining the contents of the 14 columns. The first three columns are representing the landuse name, code (which are consistent with those in “Landuse.Input” file) and type (grouping of the landuse classes). The fourth column (PFT) gives a plant-functional type code (for future use), the fifth gives the maximum height of vegetation ( $m$ ), the sixth indicates albedo (%) and the seventh indicates possible source of  $\text{NH}_x$  (0 off/1 on, currently not used). Columns 8 to 11 define the growing season (day number), column 12 and 13 lists the LAI minimum and maximum ( $m^2/m^2$ ) and columns 14 and 15 defines the length of the LAI increase and decline periods (no. of days). Finally, the last four columns give default values of foliar biomass and biogenic VOC emission potentials. See Simpson *et al.*, (2012) for details.

## 2.2.10 Stomatal conductance

Parameters for the stomatal conductance model, deposition of  $\text{O}_3$  and stomatal exchange (DO3SE) must be specified. That are based upon the ideas in Emberson *et al.*, 2000, and are discussed in Simpson and Emberson, 2006 and Tuovinen *et al.* 2004.

The ASCII file “Inputs\_DO3SE.csv” provides land-phenology data of each landuse type for stomatal conductance calculations. The data are summarised in Table 5.1 in Chapter 5 of the EMEP Status Report 1/2003 Part I (Simpson *et al.*, 2003).

The file contains a **header** with the contents of the file, with different factors needed for each of the landuse classes used in the EMEP/MSC-W model. The first two columns represent the landuse code (which are consistent with those in “Landuse.Input” file) and name. The next 22 values are different phenology factors.

## 2.2.11 Photo-dissociation rates

The photo-dissociation rates (J-values) are provided as lookup tables. The method is previously described in Jonson *et al.*, (2001). J-values are provided as clear sky, light cloud and dense cloud conditions, and the model interpolates between these according to cloudiness from the meteorological input data. In the lookup tables data are listed for every 10 degree latitude at an interval of 1 degree zenith angle at every model height.

For the two types of cloud conditions there are one **ASCII** file averaged for each season (SS); 01, 02, 03 and 04. For light cloud the four seasonal files are called “jcl1kmSS.dat”, for dense cloud conditions the four seasonal files are called “jcl3kmSS.dat”, and then for clear sky four files called “jclearSS.dat”. In addition there are two files for june called jcl1.jun and jcl3.jun.

Each file contains 18 columns. The first column is latitude of zenith angle and then the next 17 are the values for the model levels with the unit: 1/s. For more details about these rates, please read Chapter 7.2 of the EMEP Status Report 1/2003 Part I (Simpson *et al.*, 2003).

### 2.2.12 Dust files

The gridded input files “sand\_frac.dat” and “clay\_frac.dat” gives the fraction (in %) of sand and clay in the soil for each grid cell over land. The files are provided by Maxilian Posch, Netherlands Environmental Assessment Agency, CCE, personal communication.

The files are used by the module **DustProd\_ml.f90**, which calculates windblown dust emissions from soil erosion. Note that the parametrization is still in the development and testing phase, and is by default ‘turned off’. To include it in the model calculations, set USE\_DUST = .true. in “config\_emep.nml”. The user is recommended to read carefully documentation and comments in the module **DustProd\_ml.f90**.

There is also a possibility to include boundary and initial conditions for dust from Sahara. The gridded input files “DUST\_f.MM” and “DUST\_c.MM” gives monthly dust mixing ratios (MM - month, e.g. 01, 02, 03,...) for fine and coarse dust from Sahara. The files are based on calculations from a global CTM at the University of Oslo for 2000. To include Saharan dust, set USE\_SAHARA = .true. in “config\_emep.nml”.

Another source for dust is an arid surface. This is accounted for by soilmoisture calculations in **DustProd\_ml.f90**. Together with Soil Water Index from the meteorology files and permanent wilting point (pwp) from SoilTypes\_IFS.nc. This file is global and netcdf. See Simpson *et al.* (2012) section 6.10.

### 2.2.13 Site and Sonde locations for output

The model provides a possibility for extra output data of surface concentration for a set of specified measurement site locations and concentrations for the vertical column above a set of specified locations. These site and sonde locations are listed in the **ASCII** files “sites.dat” and “sondes.dat” files. These files can be changed by the user, this is described in section 3.2.

# Chapter 3

## Output files

Output files from a model run are written out in either ASCII, or (for most data outputs) in netCDF format. The different netCDF files are named after the `runlabel1` parameter set in `modrun.sh`. The model output is written to the same directory as where the runscript where submitted, as described in Chapter 4.

To check your model run, already prepared model result files can be downloaded from the EMEP/MSC-W Open Source website under “Download” section: “Model Results”. Unpacked files are placed in an output directory with model run results for a whole year and sometimes with a smaller test run for i.e. April.

Table 3.1: List of output files written in the working directory after a model run. Note: YYYY: year.

| <b>Output data files</b> | <b>Short description</b>   | <b>Format</b> |
|--------------------------|--|---------------|
| Base_day.nc              | Gridded daily values of a selection of compounds.                                      | netCDF        |
| Base_hour.nc             | Gridded hourly values of a selection of compounds.                                     | netCDF        |
| Base_month.nc            | Gridded monthly values of a selection of compounds.                                    | netCDF        |
| Base_fullrun.nc          | Gridded yearly values of a selection of compounds.                                     | netCDF        |
| sites_YYYY.cvs           | Surface daily values of a selection of stations and compounds.                         | ASCII         |
| sondes_YYYY.csv          | Vertical daily values of a selection of stations and compounds.                        | ASCII         |
| <b>Additional files</b>  | <b>Short description</b>   | <b>Format</b> |
| RunLog.out               | Summary log of runs, including total emissions of different air pollutants per country | ASCII         |
| Timing.out               | Timing log file  | ASCII         |

### 3.1 Output parameters netcdf files

Parameters to be written out Base\_day.nc, Base\_month.nc and Base\_year.nc are defined in My\_Derived\_ml.f90 and Derived\_ml.f90. In My\_Derived\_ml.f90, the user can specify the output species (air concentrations, depositions, column values), units and temporal resolution of the outputs (daily, monthly, yearly).

The name of output parameter provides some information about data. The names start with TYPE of the parameter, namely SURF (surface air concentrations), DDEP (Dry deposition), WDEP (Wet deposition), COLUMN (Vertically integrated parameters), Area (Surface area) etc.

For surface air concentrations, the general name pattern is SURF\_UNITS\_COMPONENT. Here, UNITS can e.g. be ug ( $\mu\text{g m}^{-3}$ ), ugS ( $\mu\text{g(S) m}^{-3}$ ), ugN ( $\mu\text{g(N) m}^{-3}$ ), or ppb. The user can change units in My\_Derived\_ml.f90 (in array OutputConcs). Note that the components are classified either as SPEC (species) or GROUP. The content of complex GROUP components can be found in CM\_ChemGroups\_ml.f90.

For dry depositions, given per  $1\text{m}^2$  of specified landuse, the names look like DDEP\_COMPONENT\_m2LANDUSE, where LANDUSE can be either a specific landuse type or a cell average. The units are  $\text{mg(S)m}^{-2}$  or  $\text{mg(N)m}^{-2}$ . For wet depositions, the names are WDEP\_COMPONENT, and the units are  $\text{mg(S)l}^{-1}$  or  $\text{mg(N)l}^{-1}$ .

For column integrated parameters, the names are COLUMN\_COMPONENT\_NLAYERS, where NLAYERS is the number of layers included in the integration. The units are  $\text{molec/m}^2$ , but can easily be changed in My\_Derived\_ml.f90 and Derived\_ml.f90.

VG\_COMPONENT\_LANDUSE are the dry deposition velocities on various landuse types, typically in cm/s.

Table 3.2 lists most of output parameters, providing additional explanation to the complex components. For a complete suit of currently selected output parameters, see provided output NetCDF files, or My\_Derived\_ml.f90 module.

Table 3.2: List of output parameters (not complete).

| Parameter name      | Short description   | Comments  |
|---------------------|---|---|
| SURF_ppb_O3         | O <sub>3</sub> [ppb]  |   |
| SURF_ugN_NO         | NO [ $\mu g(N)/m^3$ ]                                       | Available also in ppb   |
| SURF_ugN_NO2        | NO <sub>2</sub> [ $\mu g(N)/m^3$ ]                          | Available also in ppb   |
| SURF_ugN_HNO3       | HNO <sub>3</sub> [ $\mu g(N)/m^3$ ]                         | Available also in ppb   |
| SURF_ugN_NH3        | NH <sub>3</sub> [ $\mu g(N)/m^3$ ]                          | Available also in ppb   |
| SURF_ugS_SO2        | SO <sub>2</sub> [ $\mu g(S)/m^{-3}$ ]                       | Available also in ppb   |
| SURF_ug_SO4         | SO <sub>4</sub> <sup>2-</sup> [ $\mu g/m^3$ ]               |   |
| SURF_ug_NO3_F       | NO <sub>3</sub> <sup>-</sup> [ $\mu g/m^3$ ] fine aerosol   | As ammonium nitrate   |
| SURF_ug_NO3_C       | NO <sub>3</sub> <sup>-</sup> [ $\mu g/m^3$ ] coarse aerosol | Associated with sea salt and mineral dust                         |
| SURF_ug_TNO3        | NO <sub>3</sub> <sup>-</sup> [ $\mu g/m^3$ ] total          | Sum of fine and coarse nitrate                                    |
| SURF_ug_NH4_F       | NO <sub>4</sub> <sup>+</sup> [ $\mu g/m^3$ ] fine aerosol   | As ammonium sulphate and ammonium nitrate                         |
| SURF_ug_SIA         | SIA [ $\mu g/m^3$ ]   | Secondary Inorganic Aerosol                                       |
| SURF_ug_ECFINE      | EC fine [ $\mu g/m^3$ ]                                     | Elemental carbon  |
| SURF_ug_ECCOARSE    | EC coarse [ $\mu g/m^3$ ]                                   | Elemental carbon  |
| SURF_ug_PART_OM_F   | OM fine [ $\mu g/m^3$ ]                                     | Organic Matter fine aerosol                                       |
| SURF_ug_OMCOARSE    | OM coarse [ $\mu g/m^3$ ]                                   | Organic Matter coarse aerosol                                     |
| SURF_ug_SEASALT_F   | Sea salt fine aerosol [ $\mu g/m^3$ ]                       |   |
| SURF_ug_SEASALT_C   | Sea salt coarse aerosol [ $\mu g/m^3$ ]                     |   |
| SURF_ug_SS          | Sea salt [ $\mu g/m^3$ ]                                    | Sum of fine and coarse sea salt                                   |
| SURF_ug_DUST_ROAD_F | Road dust fine aerosol [ $\mu g/m^3$ ]                      |   |
| SURF_ug_DUST_ROAD_C | Road dust coarse aerosol [ $\mu g/m^3$ ]                    |   |
| SURF_ug_DUST_WB_F   | Windblown dust fine [ $\mu g/m^3$ ]                         |   |
| SURF_ug_DUST_WB_C   | Winblown dust coarse [ $\mu g/m^3$ ]                        |   |
| SURF_ug_DUST_SAH_F  | Saharan dust fine [ $\mu g/m^3$ ]                           | From Boundary conditions  |
| SURF_ug_DUST_SAH_C  | Saharan dust coarse [ $\mu g/m^3$ ]                         | From Boundary conditions  |
| SURF_ug_DUST_NAT_F  | Natural dust fine [ $\mu g/m^3$ ]                           | Windblown and Saharan   |
| SURF_ug_DUST_NAT_C  | Natural dust coarse [ $\mu g/m^3$ ]                         | Windblown and Saharan   |
| SURF_ug_DUST        | Mineral dust [ $\mu g/m^3$ ]                                | From all sources  |
| SURF_ug_PM10        | PM <sub>10</sub> dry mass [ $\mu g/m^3$ ]                   |   |
| SURF_ug_PM10_rh50   | PM <sub>10</sub> wet [ $\mu g/m^3$ ]                        | PM <sub>10</sub> +<br>particle water at Rh=50%                    |
| SURF_ug_PM25        | PM <sub>2.5</sub> dry [ $\mu g/m^3$ ]                       | Includes fine PM and<br>27% of coarse NO <sub>3</sub>             |
| SURF_ug_PM25_rh50   | PM <sub>2.5</sub> wet [ $\mu g/m^3$ ]                       | PM <sub>2.5</sub> +<br>particle water at Rh=50%                   |
| SURF_ug_PM25X       | PM <sub>2.5</sub> dry [ $\mu g/m^3$ ]                       | Includes fine PM and 27% of<br>coarse NO <sub>3</sub> , EC and OM |
| SURF_ug_PM25X_rh50  | PM <sub>2.5</sub> [ $\mu g/m^3$ ]                           | As PM <sub>2.5</sub> X +<br>particle water at Rh=50%              |
| SURF_ug_PMFINE      | Fine PM [ $\mu g/m^3$ ]                                     | Sum of all fine aerosols  |

*Continued on next page*

Table 3.2 – Continued from previous page

| Parameter name                   | Short description  | Comments                                    |
|----------------------------------|--|---|
| SURF_ug_PPM25                    | Primary PPM <sub>2.5</sub> [ $\mu\text{g}/\text{m}^3$ ]          | Anthropogenic emissions                     |
| SURF_ug_PPM_C                    | Primary coarse PM [ $\mu\text{g}/\text{m}^3$ ]                   | Anthropogenic emissions                     |
| SURF_ug_PM25_FIRE                | PM <sub>2.5</sub> from forest fires [ $\mu\text{g}/\text{m}^3$ ] | Sum of BC, OC<br>and rest PM <sub>2.5</sub> |
| etc.                             |  |   |
| <b>Dry Depositions</b>           |  |   |
| DDEP_SOX_m2Grid                  | Oxidized sulphur [ $\text{mg}(\text{S})/\text{m}^2$ ]            | For a grid cell<br>landuse area weighted    |
| DDEP_SOX_m2Conif                 | Oxidized sulphur [ $\text{mg}(\text{S})/\text{m}^2$ ]            | To coniferous forest                        |
| DDEP_NOX_m2Grid                  | Oxidized nitrogen [ $\text{mg}(\text{N})/\text{m}^2$ ]           | For a grid cell<br>landuse area weighted    |
| DDEP_NOX_m2Decid                 | Oxidized nitrogen [ $\text{mg}(\text{N})/\text{m}^2$ ]           | To deciduous forest                         |
| DDEP_RDN_m2Grid                  | Reduced nitrogen [ $\text{mg}(\text{N})/\text{m}^2$ ]            | For a grid cell<br>landuse area weighted    |
| DDEP_RDN_m2Seminat               | Reduced nitrogen [ $\text{mg}(\text{N})/\text{m}^2$ ]            | To semi-natural                             |
| etc.                             |  |   |
| <b>Wet Depositions</b>           |  |   |
| WDEP_PREC                        | Precipitation [mm]   |   |
| WDEP_SOX                         | Oxidized sulphur [ $\text{mg}(\text{S})/\text{l}$ ]              |   |
| WDEP_SS                          | Sea salt [ $\text{mg}/\text{l}$ ]                                |   |
| etc.                             |  |   |
| <b>Others</b>                    |  |   |
| AOD                              | Aerosol Optical Depth at 550nm                                   | Experimental                                |
| Area_Crops_Frac                  | Area fraction of crops   | Available for several landuses              |
| VG_NO3_F_Grid                    | Dry deposition velocity of fine NO <sub>3</sub> <sup>-</sup>     | Grid cell average                           |
| etc.                             |  |   |
| <b>Meteorological parameters</b> |  |   |
| USTAR_GRID                       | U grid averaged  | Available for several landuses              |
| T2m                              | Temperature at 2m [°C]   |   |
| rh2m                             | Fractional relative humidity at 2m                               |   |
| etc.                             |  |   |

## 3.2 ASCII outputs: sites and sondes

Two main options are available for the output of ASCII files for comparison with measurements or detailed model analysis. These are

**sites** output of surface concentrations for a set of specified measurement site locations.

**sondes** output of concentrations for the vertical column above a set of specified locations.

Both sites and sondes are specified and handled in similar ways, in the module **Sites\_ml.f90**, so we treat them both together below. Locations are specified in the input files “sites.dat” and “sondes.dat”. The files start with a description of its content followed by a list of the stations. For example, a sondes.dat input file may look like this:

```
# "Sondes: names, locations, elevations"
# "Area: EMEP-Europe"
# "ix: x coordinate"
# "iy: y coordinate"
# "lev: vertical coordinate (20=ground)"
: Units index
: Coords LatLong
: VertCoords EMEPsigma
: DomainName NA
#
name lat long lev #HEADERS
-   deg deg level #SKIP
#DATA:
Uccle           50.80   4.35  20 ! comment
Lerwick         60.13  -1.18  20 ! comment
Sodankyla       67.39  26.65  20 ! comment
Ny_Alesund      78.93  11.88  20 ! comment
Hohenpeissenberg 47.80  11.02  20 ! comment
```

The first line in each file is a header with file content. Then, the contents are described in more detail. Text strings after # are just clarifying comments. 'Area', e.g., is the domain to which the stations belong, e.g. 'Northern Hemisphere'.

Text after ':' is read in by the model:

- Units: either 'deg' (degrees) or 'index' (model grid indices)
- Coords: either 'LatLong' (latitudes/longitudes) or 'ModelCoords' (indices of the grid box in which the station is located)
- VertCoords: vertical coordinate system that is used in the model (usually 'EMEPsigma')

Both sites.dat and sondes.dat files are optional, but recommended. The species and meteorological data requested for site and some output are specified in **My\_Outputs.f90** by the use of arrays. Only a few met fields are defined so far but more can be added into **Sites\_ml.f90** as required.

The output files sites\_YYYY.csv, and sondes\_YYYY.csv (where YYYY are the meteorological years) are comma separated files that can be read by excel. If you include the whole year, or the 31. December, sites\_YYYY+1.csv and sondes\_YYYY+1.csv (i.e., sites\_2011.csv, and sondes\_2011.csv for the met year 2010 and so on..) are also included in the output.

# Chapter 4

## Submitting a Run

In this chapter we provide detailed information on how to run the regional EMEP/MSC-W model for two different types of simulations, namely:

**Base run** This is the default set up for yearly transport model calculations in  $50 \times 50 \text{ km}^2$  grid.

**Scenario run** A run with reduced emissions from a particular country or several countries is called a “Scenario run”. It is the basic type of run for the source-receptor calculations.

Details about the submission of these different types of runs are given below. We suggest that users test the “Base run” first, which can be done without significant changes in the code itself. One can also use the outputs of such a run in the future as a reference run for the other simulations.

## 4.1 Base run

This is an example of a minimum modrun.sh script to run the model.

```
#!/bin/bash

# Minimalistic script for run the EMEP/MSC-W model

# Link the input data
inputdir=.
ln -s $inputdir/met/* . # Driving meteorology
ln -s $inputdir/input/* . # Other input files

# Define some run parameters
trendyear=2011 # emission year
runlabel1=Base # short label
runlabel2=Opensource_setup # long label
startdate="2011 01 01" # start date (metdata)
enddate="2011 01 01" # end date (metdata)

# Put the run parameters in a temporary file
cat > INPUT.PARA << EOF
$trendyear
$runlabel1
$runlabel2
$startdate
$enddate
EOF

# Run the model
mpirun $inputdir/code/Unimod

# Clean the links to the input data and remove INPUT.PARA
ls $inputdir/met |xargs rm
ls $inputdir/input|xargs rm
rm INPUT.PARA
```

This bash shell script is designed so that users can easily adapt it to fit their needs. It contains the minimum information required to run the EMEP/MSC-W model. The script should be self-explanatory. It assumes two directories for input data. One with all the metdata for the year, and for January 1<sup>st</sup> the following year (365 +1 files), and one input directory for all the other input files. You need to set the right paths for the input directories. All the input files in the input directories are linked to the directory you are working from.

The next part of the script sets the different parameters for the model run. The trendyear can be set to change the boundary emissions for earlier and future years, see the modules **BoundaryConditions\_ml.f90** and **GlobalBCs\_ml.f90** to understand better what the trendyear setting does. The default setting is the meteorological year you are running for, in this case 2011. The runlabel1 option sets the name of the different output netCDF files, see Table 3. The startdate and enddate parameters are set for the timeperiod you want the model to run

(YYYY MM DD), and you need meteorology data for the period.

To run the model, the correct path to the EMEP/MSC-W model code has to be set (mpirun path\_to\_the\_modelcode/Unimod).

It is recommended to submit the script as a batch job. Please check the submission routine on the computer system you are running on. In the newer model versions (since 4.0) the number of nodes is set automatically from what is asked for when submitting a job. The approximate time and CPU usage is described in Section 1.2

When the job is no longer running or in the queue, it is either finished or has crashed for some reason. If the model run crashed, an error message will give information on what was missing or wrong in the routine. If the run was successful, a message

```
+++++
programme is finished
```

will be stated at the end of the log file, before printing the Timing.out file. The model results will be written to this same directory. Please make sure there is enough disk place for the model results. For more information about the model result output files, see chapter 3.

If for some reason the model crashed, please check both the log and the error file for any clue of the crash. After fixing the problem the job can be submitted again. If the model has crashed, then the links to the input data are not removed.

The script can also be submitted interactively, and either have the output written to the screen or to named error and output log files.

### 4.1.1 Model constants

In the module **ModelConstants\_ml.f90** there is a possibility to set different constants and flags when running the model. Some of these are briefly explained in Chapter 2. An example of one of these settings is shown below:

```
logical, public, parameter :: USE_CONVECTION = .false.
```

Since convection has a smaller influence on transport on higher latitudes, this flag is turned off by default when running the EECCA domain. It is however important when running the model globally. A global version of the EMEP/MSC-W model will be released later.

### 4.1.2 config\_emep.nml

The model has a namelist system. Different constants and flags are added in this file. Model gets information about running for special cases from this file. For example, this namelist sets which domain you want to run the model on, other than the default domain. The datasets provided are for the EMEP grid EECCA. It is possible to run the model on a smaller domain than the full regional model domain, as defined by x coordinates ranging from 1 to 132 and y coordinates ranging from 1 to 159.

To set a smaller domain, one needs only to specify the coordinates of the new domain in **RUNDOMAIN** in the namelist file, “config\_emep.nml”. For example:

```
!           x0  x1  y0  y1
  RUNDOMAIN = (/ 36, 100, 50, 150 /) ! smaller EECCA domain
```

tells the model to run in the domain with x coordinates ranging from 36 to 100 and y coordinates from 50 to 150.

## 4.2 Nesting

The boundary conditions needed for EMEP MSC-W model is provided with the input data. The model can read Boundary conditions data from other models as well. These data has to be in netCDF format. The boundary conditions needed for EMEP MSC-W model is provided with the input data. The model can read Boundary conditions data from other models as well. These data has to be in netCDF format.

Different Nesting modes are:

- read the external BC data only,
- produce EMEP BC data from the simulation,
- read the external BC data and produce EMEP BC data,
- using the default EMEP BC data from the input data directory and write out EMEP BC at the end of the simulation,
- read the external BC data only in the beginning of the simulation,
- read external BC at the beginning of the simulation and write out EMEP BC at the end of the simulation.

These options are controlled by the ‘**MODE**’ flag in the ‘config\_emep.nml’ file and the mode options are:

- MODE=0 → do nothing
- MODE=1 → write at given NHOURLY intervals in Nest\_ml.f90
- MODE=2 → read
- MODE=3 → read and write at given NHOURLY intervals
- MODE=10 → write at end of run
- MODE=11 → read at start
- MODE=12 → read at start and write at end

### 4.2.1 How to use External BC data (MODE=2)

Following is an example showing how to read ‘MyBC.nc’ as an external BC data. The model is reading in 3 variables **O3**, **PAN**, and **CO** from this data. See the section **&ExternalBICs\_bc**

Steps to follow:

Copy 'config\_EMEPSTD.nml' to '**config\_NEST.nml**'

Edit '**config\_NEST.nml**':

Choose the **MODE** in '**config\_NEST.nml**' file. This is done in the section **&Nest\_config**  
For egs.,

**&Nest\_config**

```
MODE          = 2                !for reading external BC
template_read_BC = 'MyBC.nc'      !(The name of your BC data file)
template_write  = 'EMEP_OUT_YYYYMMDD.nc' !(ONLY for MODE=1, 3, 10 and 12)
```

**&ExternalBICs\_config**

```
USE_EXTERNAL_BIC = T,
EXTERNAL_BIC_NAME = 'MyBICScenario' !(egs., IFS for BC data from ECMWF)
TOP_BC           = T,                !(If you want to use Top BC also from your file )
filename_eta     = 'filename.zaxis' !(This is a text file containing the
                                   description of your vertical coordinate.)
\&end
```

The checks for reading vertical levels in the BC data is done in the following order:

- The variable 'hyam' (hybrid 'a' coefficient at layer midpoint), exists :→ **eta coordinate**.
- Level is indexed with 'k' :→ **Sigma coordinate**
- 'filename\_eta' exist :→ **eta coordinate** derived from 'vct'\* information in filename\_eta
- Level indexed with 'lev' and no 'hyam' or 'filename\_eta' :→ **pressure coordinate**

Independent of the coordinates of the BC file, the BC levels will be interpolated into EMEP model levels. If the BC file level structure is not recognized, and there is no 'filename\_eta' provided, the model will crash.

An example of the 'filename\_eta' for EMEP model levels is given below. Here the 'vct' variable describes the model level boundaries in hybrid eta coordinate:

**emep\_eta.zaxis**

```
#
# zaxisID 0
#
zaxistype : surface
size      : 1
name      : sfc
longname  : surface
levels    : 0
#
# zaxisID 1
#
zaxistype = hybrid
size      : 20
name      : k
longname  : vertical sigma coordinates
```

```

units      : sigma_level
levels     : 0.0200 0.0600 0.1000 0.1425 0.1950 0.2635 0.3470
            0.4365 0.5215 0.5990 0.6695 0.7330 0.7895 0.8390
            0.8815 0.9170 0.9455 0.9670 0.9820 0.9940
vctsize    = 42
vct        =
            10000. 09600. 09200. 08800. 08350. 07750. 06980.
            06080. 05190. 04380. 03640. 02970. 02370. 01840.
            01380. 00990. 00670. 00420. 00240. 00120. 00000.
            0.0000 0.0400 0.0800 0.1200 0.1650 0.2250 0.3020
            0.3920 0.4810 0.5620 0.6360 0.7030 0.7630 0.8160
            0.8620 0.9010 0.9330 0.9580 0.9760 0.9880 1.0000

```

*\*'vct' is the vertical coordinate table describing the hybrid 'a' and 'b' values ('hyai' and 'hybi') at the layer interfaces in eta coordinate system. They must respect the following constraint:*

$$hyai_1 = 0 \quad hybi_1 = 1$$

$$hyai_0 = P_t \quad hybi_0 = 0$$

where  $P_t$  Pressure at top.

In this file, the first 21 values in 'vct' column represent 'hyai' and the rest 21 represent 'hybi' values in hPa.

&ExternalBICs\_bc

```

description='MyBICSscenario','Version name',3, ! name,version,size
map_bc=! emep,external,frac,wanted,found,IXADV,
        'O3'      , 'O3'      ,1.0,T,F,-1,
        'PAN'     , 'PAN'     ,1.0,T,F,-1,
        'CO'      , 'CO'      ,1.0,T,F,-1,
\&end

```

Variables in **map\_bc** mean the following:

1. → Variable name in EMEP MSC-W model.
2. → Variable name in the External BC data file.
3. → External BC component to EMEP component fraction.
4. → Is this component wanted or not. (should be T).
5. → Was the BC variable found on the file (reset by the model)
6. → Index of the advected model variable (reset by the model)

The fraction is helpful, when one has to map a variable that is explicitly not in EMEP model, but a fraction of that particular variable can be mapped to a matching variable in EMEP.

Caution should be given to the units of the variables in the External BC data file. The model tries to read in the variable together with its units. This is done in the module 'Units\_ml.f90'. The default units that EMEP can handle now are:

**gSm<sup>3</sup>**, **ugNm<sup>3</sup>**, **ugCm<sup>3</sup>**, **ugm<sup>3</sup>**, **ppb** and **mixing ratio (mol/mol)**.

If you have a BC data with different units, either convert them into one of the above mentioned units or add the respective conversion factor in the module 'Units\_ml.f90'.

## 4.2.2 How to produce BC data from EMEP MSC-W model (MODE=1):

The time resolution of the BC data that has to be produced by EMEP model, is specified in the module 'Nest\_ml.f90' by setting the variable 'NHOURSAVE'.

Egs., `\bf {NHOURSAVE = 3}`, means the data will be written out at 3 hour interval.

One can choose the frequency in which the BC out files has to be created (template\_write in config file), and also the domain for which the data has to be written out (sub domain part in config file). The default setup of the model creates BC data for the whole run domain.

Egs., **config\_NEST.nml**:

```
MODE = 1.
```

```
template_write = 'EMEP_OUT_YYYYMMDD.nc' (This option will write out a file
everyday with 8 timesteps in each file with the option 'NHOURSAVE=3' in Nest_ml.f90).
```

```
'EMEP_OUT_YYYYMM.nc' (will write out a file every month with no. of days of
month *8 timesteps in each file with 'NHOURSAVE=3' in Nest_ml.f90).
```

```
!----- Sub domain for write modes 1,3.
```

```
istart = 60,
```

```
jstart = 11,
```

```
iend = 107,
```

```
jend = 58,
```

This will produce a 'EMEP\_OUT' file for the domain 'i=60,107 and j=11,58'.

Please note that MODE=12 and MODE=13 will always write out fulldomain.

## 4.3 Source Receptor (SR) Runs

The EMEP/MS-CW model can be used to test the impact of reduced emission of one or more pollutants from a particular country or a number of countries. Such runs are called "Scenario runs". They are the basic runs for source-receptor calculations.

Emission factors for reduced emissions of pollutants from different sectors and countries can be defined in the input file called "femis.dat", which can be found in the downloaded input data directory, see section 2.2.6.

An example of the "femis.dat" file for a base run is shown below:

```
-----
Name  5      sox    nox    voc    nh3    pm25
27    0      1.0    1.0    1.0    1.0    1.0
-----
```

This base run example means that there are (1.0), no emission reductions of sox (SO<sub>x</sub>), nox (NO<sub>x</sub>), voc (VOC), nh3 (NH<sub>3</sub>) and pm25 (PM<sub>2.5</sub>) from all sectors in the UK.

- The first column of the second line represents the country code. (27 is the code for UK.) The codes for all countries can be found in Fortran module **Country\_ml.f90**. Please note that the country code must be the same as in the emission files for the given country.

Some countries and areas are divided into sub-areas in the emission files. In this case, one line for each sub-area has to be included into the “femis.dat” file. Countries and areas where emissions are given for sub-areas include the Russian Federation, Germany and all sea areas.

- The second column of the second line represents the sector and “0” means all sectors. Here one can write the appropriate sector code if the emission is reduced only from a specific sector. The description of each sector can also be found in the Fortran module **EmisDef\_ml.f90**.
- The columns under the pollutant names show the emission factors for the given pollutants. For example, 0.7 would mean 70% of the original emission, thus 30% reduction.
- The number (“5”) following the first text (“Name”) in the first line gives the number of pollutants treated in the file.

An example of “femis.dat” file describing 50% reduced emission of “sox” from sector 10 (the emission from agriculture) in the UK can be given as:

```
-----
Name  5   sox   nox   voc   nh3   pm25
27   10  0.5   1.0   1.0   1.0   1.0
-----
```

For a scenario run “femis.dat” file should be edited manually depending on the level of reduction one would like to test with any pollutant from any sector and/or any country. Several lines can be written in the file.

# References

- Andersson-Sköld and Simpson, 1997** Y. Andersson-Sköld and D. Simpson. Comparison of the chemical schemes of the EMEP MSC-W and the IVL photochemical trajectory models. EMEP MSC-W Note 1/97. The Norwegian Meteorological Institute, Oslo, Norway, 1997.
- Emberson et al., 2000** L. Emberson, D. Simpson, J.-P. Tuovinen, M.R. Ashmore and H.M. Cambridge. Towards a model of ozone deposition and stomatal uptake over Europe. EMEP/MSW Note 6/2000.
- Fagerli et al., 2004** H. Fagerli, D. Simpson and S. Tsyro. Unified EMEP model: Updates. In *EMEP Status Report 1/2004, Transboundary acidification, eutrophication and ground level ozone in Europe. Status Report 1/2004*, pages 11–18. The Norwegian Meteorological Institute, Oslo, Norway, 2004.
- Gardner et al., 1997** R.M. Gardner, K. Adams, T. Cook, F. Deidewig, S. Ernedal, R. Falk, E. Fleuti, E. Herms, C.E. Johnson, M. Lecht, D.S. Lee, M. Leech, D. Lister, B. Masse, M. Metcalfe, P. Newton, A. Schmitt, C. Vandenberg and R. Van Drimmelen. The ANCAT/EC global inventory of NO<sub>x</sub> emissions from aircraft. *Atmos. Environ.*, 31 (12): 1751-1766, 1997.
- Hayman et al., 2011** G.D. Hayman, R. Bergstrom, M.E Jenkin and D. Simpson, Modelling photochemical oxidants in Europe: benchmarking 7 chemical mechanisms, article in preparation, 2011,
- Jonson et al., 2001** J.E.Jonson, J.K.Sundet and L. Tarrasón. Model calculations of present and future levels of ozone and ozone precursors with a global and a regional model. *Atmos. Environ.*, 35: 525-537, 2001.
- Köhler et al., 1995** I. Köhler, R. Sausen and G. Klenner. NO<sub>x</sub> production from lightning. The impact of NO<sub>x</sub> emissions from aircraft upon the atmosphere at flight altitudes 8-15 km (AERONOX), edited by U. Schumann, final report to the Commission of the European Communities, Deutch Luft und Raumfahrt, Oberpfaffenhofen, Germany, 343–345, 1995.
- Logan, 1998** J. A. Logan. An analysis of ozonesonde data for the troposphere: Recommendations for testing 3-D models and development of a gridded climatology for tropospheric ozone. *J. Geophys. Res.*, 10 (D13):16, 115–116, 149, 1998.
- Passant, 2002** Passant NR., Speciation of UK emissions of non-methane volatile organic compounds. AEA Technology Report ENV-0545, Culham, Abingdon, United Kingdom, 2002.
- Simpson et al., 2003** D. Simpson, H. Fagerli, J.E. Jonson, S. Tsyro, P. Wind and J.-P. Tuovinen. *The EMEP Unified Eulerian Model. Model Description. EMEP MSC-W Report 1/2003*. The Norwegian Meteorological Institute, Oslo, Norway, 2003.

- Simpson and Emberson, 2006** D. Simpson and L. Emberson. Ozone fluxes – Updates. In *Transboundary Acidification, Eutrophication and Ground Level Ozone in Europe from 1990 to 2004 in support for the review of the Gothenburg Protocol. EMEP Status Report 1/2006*, pages 63–79. The Norwegian Meteorological Institute, Oslo, Norway, 2006.
- Simpson et al., 2010** Simpson, D.; Michael Gauss, S. T. & Valdebenito, Á. Model Updates Transboundary acidification, eutrophication and ground level ozone in Europe. EMEP Status Report 1/2010, The Norwegian Meteorological Institute, Oslo, Norway, 2010, 105-109
- Simpson et al., 2011** Simpson, D., Benedictow, A., Berge, H., Bergström, R. Fagerli, H., Gauss, M., Hayman, G.D., Jenkin, M.E., Jonson, J.E., Nyíri, A, Semeena, V.S, Tsyro, S., Tuovinen, J.P., Valdebenito, Á., and Wind, P., The EMEP MSC-W chemical transport model, in preparation.
- Tarrasón et al., 2004** L. Tarrasón, H. Fagerli, J.E. Jonson, H. Klein, M. van Loon, D. Simpson, S. Tsyro, V. Vestreng, P. Wind, M. Posch, S. Solberg, T. Spranger, P. Thunis and L. White. Transboundary Acidification, Eutrophication and Ground Level Ozone in Europe. EMEP Status Report 1/2004. The Norwegian Meteorological Institute, Oslo, Norway, 2004.
- Tuovinen et al., 2004** Tuovinen, J.-P.; Ashmore, M.; Emberson, L. & Simpson, D. Testing and improving the EMEP ozone deposition module *Atmos. Environ.*, 2004, 38, 2373-2385
- Wiedinmyer et al., 2011** Wiedinmyer, C., Akagi, S. K., Yokelson, R. J., Emmons, L. K., Al-Saadi, J. A., Orlando, J. J., and Soja, A. J.: The Fire INventory from NCAR (FINN): a high resolution global model to estimate the emissions from open burning, *Geosci. Model Dev.*, 4, 625641,doi:10.5194/gmd-4-625-2011, 2011