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

May 2013

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Chapter 1

Welcome to EMEP

This guide gives a brief documentation of the EMEP/MSC-W model version rv4_3. 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 pulshed 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

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
Ţ
         Chemical transport Model>
1*
!*
   Copyright (C) 2007-2012 met.no
!*
   Contact information:
!*
1*
   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
1*
     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,
1*
    but WITHOUT ANY WARRANTY; without even the implied warranty of
1*
    MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.
1*
                                                    See the
    GNU General Public License for more details.
!*
1*
    You should have received a copy of the GNU General Public License
!*
                           If not, see <http://www.gnu.org/licenses/>.
!*
     along with this program.
```

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/MSC-W has very limited resources with which to support code-usage. To help users an **EMEP Forum** is available from the EMEP/MSC-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).

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 ~ 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, pluss 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_3 are archived as a tar file. The tar file is called "EMEP_MSC-W_model.rv4_3.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_3.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

Type Filename EMEP_MSC-W_model.rv4_3.OpenSource/code Model code directory *.f90 modules files *.inc include files namelist config_emep.nml makefiles Makefile and Makefile.SRCS dependencies dependency file a copy of the license gpl.txt

Table 1.1: Contents of "EMEP_MSC-W_model.rv4_3.OpenSource.tar" file

In addition there is a run script called "modrun.sh", which will be placed in the **EMEP_MSC-W_model.rv4_3.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 50×50 km² (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 132×159 gridpoints on 50×50 km² 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 year 2010.

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 (where MM is the month). The last file for December also include a met file for January 1^{st} 2011. 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 AircraftEmis_FL.nc.

After unzipping all the meteo-tar files, the meteorology are placed under a catalogue called **EMEP_Unified_model.OpenSource2012**/. The met/ catalogue should be moved over to current version of model, for rv3_4: **EMEP_MSC-W_model.rv3_4.OpenSource**. So now there will be two directories under **EMEP_MSC-W_model.rv3_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 (NH₃, CO, NO_x, SO_x, NMVOC, PM_{2.5} and PM_{co}).

Meteorology datamet/ meteoYYYYMMDD.ncnetCDFOther Input filesinput/Global OzoneGLOBAL_O3.ncnetCDFBVOC emissionsEMEP_EuroBVOC.ncnetCDF
MeteorologymeteoYYYYMMDD.nc(365+1 files)netCDFOther Input filesinput/input/netCDFGlobal OzoneGLOBAL_O3.ncnetCDFBVOC emissionsEMEP_EuroBVOC.ncnetCDF
Other Input filesinput/Global OzoneGLOBAL_O3.ncBVOC emissionsEMEP_EuroBVOC.ncnetCDF
Other Input filesinput/Global OzoneGLOBAL_O3.ncBVOC emissionsEMEP_EuroBVOC.ncnetCDF
Global OzoneGLOBAL_O3.ncnetCDFBVOC emissionsEMEP_EuroBVOC.ncnetCDF
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 ₂ 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 emissionsDailyFac.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*
$emissplit.specials.POLL$ $ASCII^{*,\dagger}$
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 50×50 km² polar-stereographic grid projection. Vertically, the fields on 60 et a 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

Parameter	Unit	Description
3D fields - for 20 σ levels		
u, v	m/s	Horizontal wind velocity components
q	kg/kg	Specific humidity
heta	Κ	Potential temperature
CW	kg/kg	Cloud water
CL	%	3D Cloud cover
cnvuf	kg/sm^2	Convective updraft flux
cnvdf	kg/sm^2	Convective downdraft flux
PR	mm	Precipitation
2D fields - for Surface		
PS	hPa	Surface pressure
T2	Κ	Temperature at 2m height
Rh2	%	Relative humidity at 2m height
SH	W/m^2	Surface flux of sensible heat
LH	W/m^2	Surface flux of latent heat
au	N/m^2	Surface stress
SST	K	Sea surface temperature
SWC	m^{3}/m^{3}	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

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

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 depencies 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 $\mu g/m^2/h$, 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 desribed 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 $_x$ 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 "con-fig_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 **ModelConstants_ml.f90**. The model will then use 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 $\mu g/m^2$ 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 volcanoe, 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, NH₃, 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), 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) 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, NH₃, 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), 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 elleven SNAP sectors are given in the file EmisHeights.txt. The file has seven vertical levels, over the collumns 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), the second represents the sector (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. NOx includes $NO+NO_2$, and VOC can include many compounds. The information needed to retreive 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 $1^{s}t$ 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 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 64×32 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 NH_x (0 off/1 on, curently 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 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 an 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 soilmosture 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.

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

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

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 use 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 suface air concentrations, the general name pattern is SURF_UNITS_COMPONENT. Here, UNITS can e.g. be ug (μ g m⁻³), ugS (μ g(S) m⁻³), ugN (μ 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 $1m^2$ 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 $mg(S)m^{-2}$ or $mg(N)m^{-2}$. For wet depositions, the names are DDEP_COMPONENT, and the units are $mg(S)l^{-1}$ or $mg(N)l^{-1}$.

For column integrated parameters, the names are COLUMN_COMPONENT_NLAYERS, where NLAYERS is the number of layers included in the integration. The units are molec/m², 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.

Parameter name	Short description	Comments
SURF_ppb_O3	O ₃ [ppb]	
SURF_ugN_NO	$NO\left[\mu g(N)/m^3\right]$	Available also in ppb
SURF_ugN_NO2	$NO_{2} \left[\frac{\mu g(N)}{m^{3}} \right]$	Available also in ppb
SURF_ugN_HNO3	$\frac{1}{1} \frac{1}{\mu g(N)/m^3}$	Available also in ppb
SURF ugN NH3	$NH_2 \left[\mu g(N) / m^3 \right]$	Available also in ppb
SUBF ugS SO2	$SO_2 \left[\frac{\mu g(S)}{m^{-3}} \right]$	Available also in ppb
50101-485-502	502[rivanable also in pps
SURF ug SO4	$SO_4^{2-} [\mu g/m^3]$	
SURF ug NO3 F	NO_2^- [µg/m ³] fine aerosol	As ammonium nitrate
SUBF ug NO3 C	NO_{2}^{-} [µg/m ³] coarse aerosol	Associated with sea salt and
20101-08-1100-0		mineral dust
SURF ug TNO3	$NO_{2}^{-} \left[\mu g/m^{3} \right]$ total	Sum of fine and coarse nitrate
SUBF ug NH4 F	NO^+_{+} [µq/m ³] fine aerosol	As ammonium sulphate and
		ammonium nitrate
SUBE ug SIA	SIA $\left[\mu q/m^3\right]$	Secondary Inorganic Aerosol
SOM _ug_SIA	$SIA\left[r^{\prime}/m^{\prime}\right]$	Secondary morganic Aerosor
SUBE 110 ECFINE	EC fine $\left[\frac{\mu g}{m^3}\right]$	Elemental carbon
SUBF ug ECCOABSE	EC coarse $\left[\frac{\mu q}{m^3}\right]$	Elemental carbon
SUBF ug PART OM F	$\frac{1}{100} \frac{1}{100} \frac{1}$	Organic Matter fine aerosol
SUBE ug OMCOARSE	$OM \text{ coarso } \left[\frac{\mu q}{m^3} \right]$	Organic Matter mic acrosol
SOULT - ug_OMOOAIUSE	$\operatorname{OM}\left[\operatorname{Coarse}\left[\operatorname{Ps}/\operatorname{m}^{2}\right]\right]$	Organic Matter Coarse acrosor
SURF ug SEASALT F	Sea salt fine aerosol $\left[\mu g/m^3\right]$	
SUBF ug SEASALT C	Sea salt coarse aerosol $[\mu g/m^3]$	
SUBF ug SS	Sea salt $[\mu g/m^3]$	Sum of fine and coarse sea salt
SUBF ug DUST BOAD F	Boad dust fine aerosol $\left[\frac{\mu q}{m^3}\right]$	Sum of the and course sea sait
SUBF ug DUST BOAD C	Road dust coarse aerosol $[\mu g/m^3]$	
SUBE ug DUST WB F	Windblown dust fine $\left[\frac{\mu q}{m^3}\right]$	
SUPE ug DUST WB C	Winblown dust nine $[P^{g}/m^{2}]$	
SURF_ug_DUST_WB_C	Soboron dust fine $\left[\frac{\mu g}{3}\right]$	From Boundary conditions
SURF_ug_DUST_SAILF	Saharan dust nine $[\mu g/m^3]$	From Doundary conditions
SURF_ug_DUST_SAR_C	Sanarah dust coarse $\left[\frac{\mu g}{m^3}\right]$	Windhlerm and Calanan
SURF_Ug_DUS1_NA1_F	Natural dust fine $\left[\mu g/m^3\right]$	Windblown and Sanaran
SURF_ug_DUS1_NA1_C	Natural dust coarse $\left[\frac{\mu y}{m^3}\right]$	Windblown and Sanaran
SURF_ug_DUST	Mineral dust $\left[\frac{\mu g}{m^3}\right]$	From all sources
SURF ug PM10	$PM_{10} dry mass[ua/m3]$	
SURF_ug_I MI0	$I M_{10} \text{ ury } \text{mass}[r^g/m^s]$ DM wet $[ug/3]$	DM
SURF_ug_FM10_III50	ΓM_{10} wet $\left[\frac{\mu g}{m^{0}}\right]$	$\Gamma M_{10} +$
CLIDE no DM95	$DM = dmr \left[\mu q / 3 \right]$	Includes free DM and
SURF_ug_PM25	$PM_{2.5} \text{ dry } [\mu g/m^3]$	270° of source NO
CUDE DMOT 150	$\mathbf{DM} = \mathcal{A} \left[u_0 / 2 \right]$	27% of coarse NO_3
SURF_ug_PM25_rh50	$PM_{2.5}$ wet $\left[\frac{\mu g}{m^3}\right]$	$PM_{2.5} +$
		particle water at $Rh=50\%$
SURF_ug_PM25X	$PM_{2.5} dry [\mu g/m^3]$	Includes fine PM and 27% of
		coarse NO_3 , EC and OM
SURF_ug_PM25X_rh50	$PM_{2.5} \ [\mu g/m^3]$	As $PM_{2.5}X +$
		particle water at $Rh=50\%$
SURF_ug_PMFINE	Fine PM $\left[\frac{\mu g}{m^3}\right]$	Sum of all fine aerosols
		Continued on next page

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

Table $3.2 - Continued$ from previous page						
Parameter name	Short description	Comments				
$SURF_ug_PPM25$	Primary $PPM_{2.5} \left[\frac{\mu g}{m^3} \right]$	Anthropogenic emissions				
$SURF_ug_PPM_C$	Primary coarse PM $\left[\frac{\mu g}{m^3}\right]$	Anthropogenic emissions				
SURF_ug_PM25_FIRE	$PM_{2.5}$ from forest fires $\left[\frac{\mu g}{m^3}\right]$	Sum of BC, OC				
		and rest $PM_{2.5}$				
etc.						
	Dry Depositions					
DDEP_SOX_m2Grid	Oxidized sulphur $[mg(S)/m^2]$	For a grid cell				
	, _	landuse area weighted				
DDEP_SOX_m2Conif	Oxidized sulphur $\left[\frac{mg(S)}{m^2}\right]$	To coniferous forest				
DDEP_NOX_m2Grid	Oxidized nitrogen $[mg(N)/m^2]$	For a grid cell				
		landuse area weighted				
DDEP_NOX_m2Decid	Oxidized nitrogen $[mg(N)/m^2]$	To decideous forest				
DDEP_RDN_m2Grid	Reduced nitrogen $[mg(N)/m^2]$	For a grid cell				
		landuse area weighted				
DDEP_RDN_m2Seminat	Reduced nitrogen $[mg(N)/m^2]$	To semi-natural				
etc.	<u> </u>					
	Wet Depositions					
WDEP_PREC	Precipitation [mm]					
WDEP_SOX	Oxidized sulphur $[mg(S)/l]$					
WDEP_SS	Sea salt $[mg/l]$					
etc.						
	Others					
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_3^-	Grid cell average				
etc.	· - · · ·	2				
	Meteorological parameters					
USTAR_GRID	U grid averaged	Available for several landuses				
T2m	Temperature at $2m [^{\circ}C]$					
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:
                   50.80
Uccle
                            4.35
                                   20
                                       ! comment
Lerwick
                   60.13
                           -1.18
                                   20
                                       !
                                         comment
Sodankyla
                   67.39
                           26.65
                                   20
                                       1
                                         comment
Ny_Alesund
                   78.93
                           11.88
                                   20
                                       1
                                         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 sone 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_2010.csv and sondes_2010.csv are comma separated files that can be read by excel. If you include the whole year, or the 31. December, sites_2011.csv and sondes_2011.csv are also incued 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
                            # Other input files
ln -s $inputdir/input/* .
# Define some run parameters
trendyear=2010
                            # emission year
runlabel1=Base
                            # short label
runlabel2=Opensource_setup # long label
startdate="2010 01 01"
                            # start date (metdata)
                            # end date (metdata)
  enddate="2010 01 01"
# 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 contain 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 2010, and for January 1^{st} 2011 (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 **Bound-aryConditions_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 2010. 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

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 \rightarrow do nothing
- MODE=1 \rightarrow write at given NHOURSAVE intervals in Nest_ml.f90
- MODE= $2 \rightarrow \text{read}$
- MODE=3 \rightarrow read and write at given NHOURSAVE intervals
- MODE=10 \rightarrow write at end of run
- MODE=11 \rightarrow read at start
- MODE=12 \rightarrow 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)

$\& External BICs_config$

\&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 : \rightarrow eta coordinate.
- Level is indexed with 'k' :— Sigma coordinate
- 'filename_eta' exist : \rightarrow eta coordinate derived from 'vct'* information in filename_eta
- Level indexed with 'lev' and no 'hyam' or 'filename_eta' : \rightarrow 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
          : 1
size
          : sfc
name
longname : surface
levels
          : 0
#
# zaxisID 1
#
zaxistype = hybrid
          : 20
size
          : k
name
         : vertical sigma coordinates
longname
```

```
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
          = 42
vctsize
          _
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:

```
\begin{array}{l} hyai_1 = 0 \ hybi_1 = 1 \\ hyai_0 = P_t \ hybi_0 = 0 \\ where \ P_t \ Pressure \ at \ top. \end{array}
```

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

&ExternalBICs_bc

\&end

Variables in **map_bc** mean the following:

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

gSm³, ugNm³, ugCm³, ugm³, 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 produced by EMEP model, is specifed 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.
                 = 'EMEP_OUT_YYYYMMDD.nc' (This option will write out a file
template_write
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/MSC-W 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_x), nox (NO_x), voc (VOC), nh3 (NH₃) and pm25 (PM_{2.5}) 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.

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