

# The Unified EMEP Model - User's Guide

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# Chapter 1

## Welcome to EMEP

This guide gives a brief documentation of the EMEP/MSC-W model version rv4.0. 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 Open Source website:  
<https://wiki.met.no/emep/page1/unimodopensource>

## 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 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 Unified EMEP/MS-CW 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 ~3.5 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/MS-CW model User Guide before you start downloading anything from the EMEP Open Source website.

Please register as an EMEP User on the **EMEP Forum** (EMEP Open Source website under “Users” section: “EMEP Forum”) before you start downloading the EMEP/MS-CW 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/MS-CW model:

- Register as an EMEP User
- Read the EMEP/MS-CW model User Guide
- Download input data (description in Chapter 2 and data available from the EMEP Open Source website under “Download” section: “Input Data”)
- Download the EMEP/MS-CW model source code (description in section 1.4 and the files are available from the EMEP 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 Open Source website under “Download” section: “Model Results”.

## 1.4 Model code

The EMEP/MSC-E model code version rv.4.0 are archived as a tar file. The tar file is called “EMEP\_Unified\_model.tar.bz” and is downloadable from the EMEP Open Source website.

Once this file is untarred all model files needed for a model run will be found under the directory **EMEP\_Unified\_model.OpenSource2012/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\_Unified\_model.tar” file

Type	Filename
<b>Model code directory</b>	EMEP_Unified_model.OpenSource2012/code
modules files	*.f90
include files	*.inc
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\_Unified\_model.OpenSource2012/** 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  $50 \times 50 \text{ km}^2$  (at  $60^\circ\text{N}$ ) 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 **ModelConstants\_ml.f90** module.

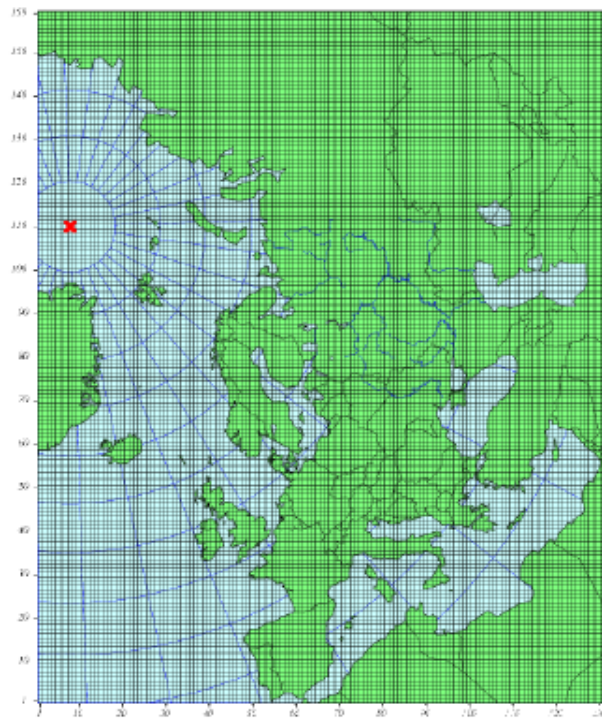


Figure 1.1: The extended EMEP grid covering EECCA area with  $132 \times 159$  gridpoints on  $50 \times 50 \text{ km}^2$  resolution defined on a polarstereographic projection.



# 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 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<sup>st</sup> 2011. The last zipped input file (called other\_input\_files.tar.bz2) contains all other input files needed for running the EMEP model, except AircraftEmis\_FL.nc. After unzipping all of the tar files, there will be two directories under EMEP\_Unified\_model.OpenSource2012. All the meteorology are placed under /met, and the rest of the input files under /input. All the files, both meteorological and the other input files, are described in this chapter.

**IMPORTANT:** The input data available in the EMEP 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.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	ForestFire_Emis_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	HAURLY-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 Unified EMEP 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 Mmoisture index level 1
$SMI3$		Soil Mmoisture index level 3

### 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 for v.2011-06 (last OpenSource version). 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, “Landuse.PS.5km.nc“ 5 km resolution landuse over the EMEP domain, and a global “LanduseGLC.nc” where the previous file is not defined. The different landuse types are described in Simpson *et al.* (2012).

### 2.1.5 Degree-day factor

The degree-day files give the daily factors to be applied to SNAP-2, using degree-days calculated from the gridded temperature fields. See Simpson *et al.* (2012) section 6.1.2.

### 2.1.6 $\text{NO}_x$ depositions

The file `annualNdep.nc` is a map of N-deposition pre-calculated by the EMEP MSC-W model for a 5-year period. This map is used as an input to the soil-NO calculations (areas with high deposition loads have greater soil-NO emissions).

### 2.1.7 Road Dust

Dust formed from road traffic can now be included as particles in the EMEP model. `USE_ROADDUST` has to be set to `.true.` in `ModelConstants_ml.f90`. There are two files needed with road dust, `RoadMap.nc` and `AVG_SMI_2005-2010.nc`. The module `Emissions_ml.f90` handles road dust emissions.

### 2.1.8 Aircraft emissions

In the EMEP/MS-CW 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 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

There is a possibility to include emissions by Forest Fires. By setting `USE_FOREST_FIRES = .true.` in `ModelConstants_ml.f90`, and getting forest fire data from <http://bai.acd.ucar.edu/Data/fire/>. Register and download the 2010 GEOS-chem daily data. The data are read in by `ForestFire_ml.f90`, and the downloaded data have to be stored in an netCDF file compatible with this 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 Unified EMEP model consists of gridded annual national emissions based on emission data reported every year to EMEP/MSW (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.

Version rv4.0 also includes hourly time factors for pollutants. 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.

### 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 “lt21-nox.datMM”.

## 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 **ModelConstants\_ml.f90**. 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 **ModelConstants\_ml.f90**.

Another source for dust is an arid surface. This is accounted for by soil moisture 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, the Runlog output, and the zipped sites and sondes files are named after the `runlabel1` parameter set in `modrun.sh`. The model output is written to the same directory as where you submitted your run with the `modrun.sh` script, as described in Chapter 4.

To compare you you model results, there has been made available model result files that can be downloaded from the EMEP Open Source website under “Download” section: “Model Results”. There are both model results for a run over a whole year, and a test run over two days from January 1<sup>st</sup> to 2<sup>nd</sup>. These are placed in an `output/` directory.

Table 3.1: List of output files written in the working directory after a model run. Note: YY: year, MM: month.

<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.csv	Surface daily values of a selection of stations and compounds.	ASCII
sondes.csv	Vertical daily values of a selection of stations and compounds.	ASCII
<b>Additional files</b>	<b>Short description</b>	<b>Format</b>
Base_RunLog	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 [ $\mu\text{g}^{(N)}/\text{m}^3$ ]	Available also in ppb
SURF_ugN_NO2	NO <sub>2</sub> [ $\mu\text{g}^{(N)}/\text{m}^3$ ]	Available also in ppb
SURF_ugN_HNO3	HNO <sub>3</sub> [ $\mu\text{g}^{(N)}/\text{m}^3$ ]	Available also in ppb
SURF_ugN_NH3	NH <sub>3</sub> [ $\mu\text{g}^{(N)}/\text{m}^3$ ]	Available also in ppb
SURF_ugS_SO2	SO <sub>2</sub> [ $\mu\text{g}^{(S)}/\text{m}^{-3}$ ]	Available also in ppb
SURF_ug_SO4	SO <sub>4</sub> <sup>2-</sup> [ $\mu\text{g}/\text{m}^3$ ]	
SURF_ug_NO3_F	NO <sub>3</sub> <sup>-</sup> [ $\mu\text{g}/\text{m}^3$ ] fine aerosol	As ammonium nitrate
SURF_ug_NO3_C	NO <sub>3</sub> <sup>-</sup> [ $\mu\text{g}/\text{m}^3$ ] coarse aerosol	Associated with sea salt and mineral dust
SURF_ug_TNO3	NO <sub>3</sub> <sup>-</sup> [ $\mu\text{g}/\text{m}^3$ ] total	Sum of fine and coarse nitrate
SURF_ug_NH4_F	NO <sub>4</sub> <sup>+</sup> [ $\mu\text{g}/\text{m}^3$ ] fine aerosol	As ammonium sulphate and ammonium nitrate
SURF_ug_SIA	SIA [ $\mu\text{g}/\text{m}^3$ ]	Secondary Inorganic Aerosol
SURF_ug_ECFINE	EC fine [ $\mu\text{g}/\text{m}^3$ ]	Elemental carbon
SURF_ug_ECCOARSE	EC coarse [ $\mu\text{g}/\text{m}^3$ ]	Elemental carbon
SURF_ug_PART_OM_F	OM fine [ $\mu\text{g}/\text{m}^3$ ]	Organic Matter fine aerosol
SURF_ug_OMCOARSE	OM coarse [ $\mu\text{g}/\text{m}^3$ ]	Organic Matter coarse aerosol
SURF_ug_SEASALT_F	Sea salt fine aerosol [ $\mu\text{g}/\text{m}^3$ ]	
SURF_ug_SEASALT_C	Sea salt coarse aerosol [ $\mu\text{g}/\text{m}^3$ ]	
SURF_ug_SS	Sea salt [ $\mu\text{g}/\text{m}^3$ ]	Sum of fine and coarse sea salt
SURF_ug_DUST_ROAD_F	Road dust fine aerosol [ $\mu\text{g}/\text{m}^3$ ]	
SURF_ug_DUST_ROAD_C	Road dust coarse aerosol [ $\mu\text{g}/\text{m}^3$ ]	
SURF_ug_DUST_WB_F	Windblown dust fine [ $\mu\text{g}/\text{m}^3$ ]	
SURF_ug_DUST_WB_C	Winblown dust coarse [ $\mu\text{g}/\text{m}^3$ ]	
SURF_ug_DUST_SAH_F	Saharan dust fine [ $\mu\text{g}/\text{m}^3$ ]	From Boundary conditions
SURF_ug_DUST_SAH_C	Saharan dust coarse [ $\mu\text{g}/\text{m}^3$ ]	From Boundary conditions
SURF_ug_DUST_NAT_F	Natural dust fine [ $\mu\text{g}/\text{m}^3$ ]	Windblown and Saharan
SURF_ug_DUST_NAT_C	Natural dust coarse [ $\mu\text{g}/\text{m}^3$ ]	Windblown and Saharan
SURF_ug_DUST	Mineral dust [ $\mu\text{g}/\text{m}^3$ ]	From all sources
SURF_ug_PM10	PM <sub>10</sub> dry mass [ $\mu\text{g}/\text{m}^3$ ]	
SURF_ug_PM10_rh50	PM <sub>10</sub> wet [ $\mu\text{g}/\text{m}^3$ ]	PM <sub>10</sub> + particle water at Rh=50%
SURF_ug_PM25	PM <sub>2.5</sub> dry [ $\mu\text{g}/\text{m}^3$ ]	Includes fine PM and 27% of coarse NO <sub>3</sub>
SURF_ug_PM25_rh50	PM <sub>2.5</sub> wet [ $\mu\text{g}/\text{m}^3$ ]	PM <sub>2.5</sub> + particle water at Rh=50%
SURF_ug_PM25X	PM <sub>2.5</sub> dry [ $\mu\text{g}/\text{m}^3$ ]	Includes fine PM and 27% of coarse NO <sub>3</sub> , EC and OM
SURF_ug_PM25X_rh50	PM <sub>2.5</sub> [ $\mu\text{g}/\text{m}^3$ ]	As PM <sub>2.5</sub> X + particle water at Rh=50%
SURF_ug_PMFINE	Fine PM [ $\mu\text{g}/\text{m}^3$ ]	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 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 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 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 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\_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 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=2010 # emission year
runlabel1=Base # short label
runlabel2=Opensource_setup # long label
startdate="2010 01 01" # start date (metdata)
enddate="2010 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 2010, and for January 1<sup>st</sup> 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 **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 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 Unified EMEP 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 new model version (4.0) the number of nodes is set automatically from what is asked for when submitting a job. However there is a minimum limit of 4. 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 stating

```
+++++
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/MS-CW model will be released later.

The module also sets which domain you want to run the model on. The datasets provided are for the new 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 Fortran module **ModelConstants\_ml.f90**. For example:

```

!           x0   x1  y0   y1
RNDOMAIN = (/ 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 Scenario run

The EMEP 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.

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