

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

July 2011

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Chapter 1

Welcome to EMEP

This guide gives a brief documentation of the EMEP/MSC-W model version v.2011-06. 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.

Documentation for this version of the model is currently (July 2011) being written up for submission to the EMEP special issue in the journal *Atmos. Chem. and Physics*. This paper will be referred to as Simpson et al. (2011) in this manual, and if accepted links provided on the EMEP web-page. The provisional title and author list is:

- Simpson, D., Benedictow, A., Berge, H., Bergström, R. Fagerli, H., Gauss, M., Hayman, G.D., Jenkin, M.W., Jonson, J.E., Nyíri, A, Semeena, V.S, Tsyro, S., Tuovinen, J.P., Valdebenito, Á., and Wind, P., The EMEP MSC-W chemical transport model.

The main documentation for the older version of the model is still relevant and is given in:

- D. Simpson, H. Fagerli, J.E. Jonson, S. Tsyro, P. Wind, and J.-P. Tuovinen. The Unified EMEP Eulerian Model. Model Description. EMEP MSC-W Report 1/2003, The Norwegian Meteorological Institute, Oslo, Norway, 2003.
- H. Fagerli and D. Simpson and S. Tsyro, in EMEP Status Report 1/2004 (Tarrason, L. *et al.*), Transboundary acidification, eutrophication and ground level ozone in Europe, Status Report 1/2004, Chapter 2 (pp 11-18), The Norwegian Meteorological Institute, Oslo, Norway, 2004.

with a summary of recent changes given in:

- Simpson, D.; Michael Gauss, S. T. & Valdebenito, Á. Model Updates Transboundary acidification, eutrophication and ground level ozone in Europe. EMEP Status Report 1/2010, The Norwegian Meteorological Institute, Oslo, Norway, 2010, 105-109

Copies of these reports can be obtained from the EMEP website:

<http://www.emep.int>, and a HTML copy of EMEP Status Report 1/2003 is available at <http://www.emep.int/UniDoc/index.html>

The model source code is available from the EMEP Open Source website:

<http://www.emep.int/OpenSource/index.html>

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) 2007-2011 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 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).

1.2 Computer Information

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

Fortran 95 compiler

NetCDF Library (>3.5.1)

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/MSC-E 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/MSC-E 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-E model:

- Register as an EMEP User
- Read the EMEP/MSC-E 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/MSC-E 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”.
- If wanted, download some helper programmes to read site and sonde outputs, see sections 1.5,3.1. The files are available from the EMEP Open Source website under “Download” section: “Tools”.

1.4 Model code

The EMEP/MSC-E model code version v.2011-06 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.OpenSource2011/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
Model code directory	EMEP_Unified_model.OpenSource2011/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.OpenSource2011/** 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 Helper tools

For users interested in reading the ascii site and sonde specific outputs, two help programmes (Rd_sites.f90, Rd_sondes.f90) are provided, in the **EMEP_Unified_model.OpenSource2011/tools** directory. These programmes are readily compiled with e.g. gfortran, and can be run without arguments to obtain usage instructions. See section 3.1 for more details.

1.6 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°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.

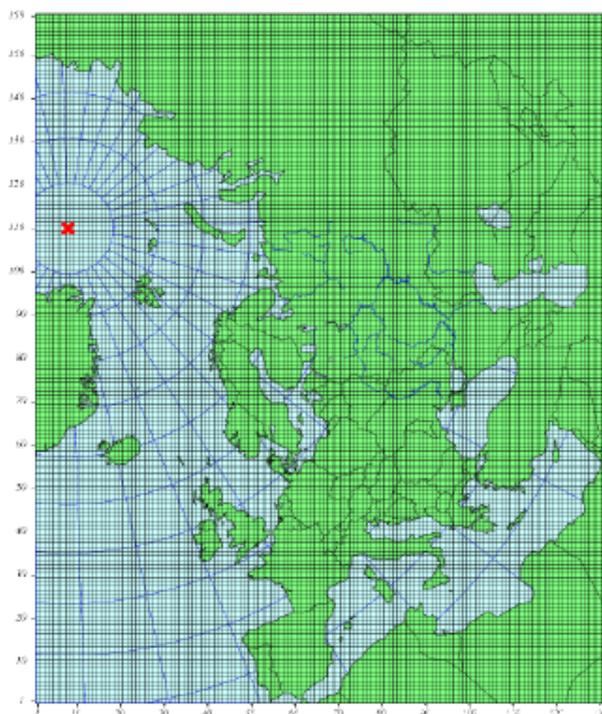


Figure 1.1: The extended EMEP grid covering EECCA area with 132×159 gridpoints on $50 \times 50 \text{ km}^2$ resolution defined on a polarstereographic projection.

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 2008.

The input files are zipped in 13 different files. There are 12 zipped files for the meteorology, one for each month, called meteo2008MM.tar.bz2 (where MM is the month). The last file for December also include a met file for January 1st 2009. 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.OpenSource2011. 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 (NH₃, CO, NO_x, SO_x, NMVOC, PM_{2.5} and PM_{co}).

Data	Name	Format
Meteorology data	met/	
Meteorology	meteoYYYYMMDD.nc (366+1 files)	netCDF
Other Input files	input/	
Global Ozone	GLOBAL.O3.nc	netCDF
BVOC emissions	EMEP_EuroBVOC.nc	netCDF
Aircraft emissions	AircraftEmis_FL.nc	netCDF†
Surface Pressure	SurfacePressure.nc	netCDF†
Landuse	Inputs.Landuse	ASCII*
Land/Sea mask	landsea_mask.dat	ASCII
Natural SO ₂	natso2MM.dat (12 files)	ASCII
Volcanoes	VolcanoesLL.dat	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
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†
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/MS-CW 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/MS-CW Model

Parameter	Unit	Description
3D fields - for 20 σ levels		
u, v	m/s	Wind velocity components
q	kg/kg	Specific humidity
$\dot{\sigma}$	s^{-1}	Vertical wind in σ coordinates
θ	K	Potential temperature
CL	%	3D Cloud cover
PR	mm	Precipitation
CW	kg/kg	Cloud water
2D fields - for Surface		
PS	hPa	Surface pressure
$T2$	K	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
τ	N m^{-2}	Surface stress
SST	K	Sea surface temperature
SWC	m^3/m^3	Soil water content*
$DSWC$	m^3/m^3	Deep soil water content*
$sdepth$	m	Snow depth
ice	%	Fraction of ice

Notes: * not yet used

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. The new approach is documented in Simpson *et al.*, 2011.

2.1.4 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 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.

2.1.5 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 al-

ready 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.

2.2 ASCII files

2.2.1 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 is a **header** in the file that contains short abbreviations for the different land cover types, e.g. CF for temperate/boreal coniferous forest. The landuse types are summarized in Table 5.1 in Chapter 5 of the EMEP Status Report 1/2003 Part I (Simpson *et al.*, 2003).

The different landuse types are given as a percentage of area for each EMEP grid cell in the **ASCII file** “Inputs.Landuse”.

2.2.2 Land/Sea mask

This file, based on the meteorological model’s roughness length, is used to assign a land/sea mask within the Unified EMEP model, since there is a need to modify the stability information for coastal grid cells (which contain land, but is not resolved by the NWP model supplying meteorological data to the Unified EMEP model).

The gridded **ASCII file** “landsea_mask.dat” contains 3 columns. The first two columns represent the ‘i’ and ‘j’ indices of the EECCA grid and the third column gives the class of the grid cell, where the EMEP model use 0 for ocean, and ≥ 1 as land.

2.2.3 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.

2.2.4 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 kttons per year in column 4.

2.2.5 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/MS-CW (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

2.2.6 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.

2.2.7 Emission factor for scenario runs

Scenario run in the case of the EMEP/MS-CW 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.

2.2.8 Chemical speciation of emissions

Many of the emission files give emissions of a group of compounds, e.g. NO_x includes NO+NO₂, 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 1st 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.

2.2.9 Lightning emissions

Emissions of NO_x from lightning are included in the model as monthly averages on a T21 (5.65°×5.65°) 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 "lt21-nox.datMM".

2.2.10 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, 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., 2011 for details.

2.2.11 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.

2.2.12 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).

2.2.13 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**.

2.2.14 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 3.1.

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 1st to 2nd. 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.

Output data files	Short description	Format
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.MMY	Surface daily values of a selection of stations and compounds per month.	ASCII
sondes.MMY	Vertical daily values of a selection of stations and compounds per month.	ASCII
Additional files	Short description	Format
Base_RunLog	Summary log of runs, including total emissions of different air pollutants per country	ASCII
Timing.out	Timing log file	ASCII

3.1 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: Northern Hemisphere"
# "latitude in degrees (positive north)"
# "longitude in degrees (positive east of Greenwich)"
: Units deg
: Coords LatLong
: VertCoords EMEPsigma
: DomainName Hemis
#
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
```

Or, in cases where grid indices are used rather than latitudes and longitudes. This is useful if you want sites and sonde output from a line or an area from the model.

```
# "Sites: names, locations, elevations"
# "Area: EMEP-EECCA"
# "ix: x coordinate"
# "iy: y coordinate"
# "lev: vertical coordinate (20=ground)"
: Units index
: Coords ModelCoords
: VertCoords EMEPsigma
: DomainName EMEP-50kmEECCA
#
name ix iy lev #HEADERS
-   index index level #SKIP
#DATA:
```

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')
- DomainName: domain, for which the model is run (e.g. 'Global_1x1' or 'Hemis')

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 outputs consist of a header giving the number of sites requested, species/met data requested, and then the actual values for each variable for each station. For the sonde data values are given for all 20 levels, starting with the ground-level values. These files are best read using some helper programmes, which we provide in the "Tools" directory:

Rd_sites.f90 - reads the sites output file for one month, and allows the user to select site and component. Produces several outputs (SITES.hrly etc.), including hourly values, daily mean and max. The code is quite short and easy to modify

Rd_sondes.f90 - similar to Rd_sites, but for the sondes output.

Simply compile and run the executable to obtain usage instructions.

3.2 NetCDF outputs, Derived fields

The netCDF output files can contain both 2D and 3D data fields. The module **Derived_ml.f90** contains an extensive set of predefined outputs, and others are defined as required in **My_Derived_ml.f90**. The user may choose which of these possible data fields should be written into the output files by modifying the module called **My_Derived_ml.f90**.

Most data fields are defined by the array OutputConcs. A defined output field for ozone in ppb is for example given as:

```
typ_s5i("O3          ", "ppb", D2,"AIR_CONCS", SPEC, D),&
```

This will give a 'SURF_ppb-O3' 2-dimensional surface field in the output netCDF file for the fullrun, monthly and daily output. Setting the dimensions to D3 will give an additional 3-dimensional field.

Other arrays where output fields are given are D2_SR, D2_EXTRA, VEGO3_WANTED and WDEP_WANTED. Other fields are also defined in **My_Derived_ml.f90** e.g. for dry depositions, emissions, canopy etc.

Note that by default the maximum field of 2- and 3-dimensional output field are restricted to 200 and 5 respectively. These can be changed with MAX_NUM_DERIV2D and MAX_NUM_DERIV3D in **My_Derived_ml.f90** .

The output frequency is set in **Derived_ml.f90** , for example for the surface fields:

```
call AddNewDeriv( "PSURF ", "PSURF", "SURF","-", "hPa", &
                 -99, -99, F, 1.0, T, IOU_DAY )
```

Where the IOU_DAY setting gives the field in the fullrun.nc, month.nc in addition to the day.nc model output files. IOU_MON gives the field in the fullrun.nc and the month.nc file.

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 50×50 km² 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=2008 # emission year
runlabel1=Base # short label
runlabel2=Opensource_setup # long label
startdate="2008 01 01" # start date (metdata)
enddate="2008 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 2008, and for January 1st 2009 (366 +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 2008. 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. When setting the number of nodes, it is important that it equals to the number set in the FORTRAN module **ModelConstants_ml.f90**. In the module you set the wanted nodes in the x- and y-direction with **NPROCX** and **NPROCY**. The product of these two is the number of nodes used. 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. There is an output log file and error file written to the directory where your `modrun.sh` script is residing. 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 **ModelConstants_ml.f90** also sets the number of processors used in each direction with **PROCX** and **NPROCY**. As described above, it is important that the product of these match the number set when submitting the job.

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
  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 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 2.2.7.

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 (NH_3) and pm25 ($\text{PM}_{2.5}$) 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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