# The Unified EMEP Model - User Guide

October 10, 2008

# Chapter 1 Welcome to EMEP

This guide gives a brief documentation of the Unified EMEP model version rv.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. This guide is also intended to give some advice on new programming with a few simple ideas and rules.

The main documentation for the model 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.

Copies of both 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>
I.
!*
!*
   Copyright (C) 2007 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
1*
!*
     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
1*
     MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.
                                                      See the
!*
     GNU General Public License for more details.
!*
1*
     You should have received a copy of the GNU General Public License
!*
!*
     along with this program. If not, see <a href="http://www.gnu.org/licenses/">http://www.gnu.org/licenses/</a>>.
```

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. An **EMEP** Forum is set up and are available from the EMEP Open Source website in section "Users": "EMEP Forum" to help users, and hopefully to let users help other users. 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 model you need:

Fortran 95 compiler NetCDF Library (>3.5.1) MPI Library (>1.)

It is necessary to compile with double precision reals (8 bytes reals). The program has been tested with PGI 6.0 and Intel compilers on x86 platforms, an Intel compiler on an Itanium2 cluster, and with an XL compiler on a power5+ cluster; examples of Makefiles are provided with the model code source files.

The code has been tested with 1 to 128 CPU, and scales well. If only one CPU is used 1-2 GB memory is required and if more than one for example 32 CPU are used, 200 MB of memory per CPU is enough (in the case of a 170X133 grid size). It takes  $\sim 4.5$  hrs on 32 Opteron 246 (2GHz) for 1 year.

When downloading input data in order to do a "base run" please make sure that there are 19 Gb disc space available, especially due to large meteorology input files.

## **1.3** Getting Started

It recommended to read all the chapters of this Unified EMEP 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 Unified EMEP 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 Unified EMEP model:

- Register as an EMEP User
- Read the Unified EMEP 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 Unified EMEP model source code (description in section 1.4 and the files are available from the EMEP Open Source website under "Download" section: "Model Cod")
- Follow the instructions for 'Submitting a Run' (description in Chapter 4 and/or on the EMEP Open Source website under "Documentation" section: "Submitting a run")
- 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 Unified EMEP model code version rv3 are archived into a tar file. The tar file is called "EMEP\_Unified\_model.tar" and is downloadable from the EMEP Open Source website.

All model files needed for a model run will be found under the directory **Unify/Unimod.rv3**/ where the model source code, makefiles, the runscript and a copy of the license file are stored, once this tar file is untarred. An overview is given in Table 1.1

Type	Filename
Model code directory	Unify/Unimod.rv3
modules files	*.f90
include files	*.inc
makefiles	Makefile_*
run script	modrun.pl
a copy of the licence	gpl.txt

Table 1.1: Contents of "EMEP\_Unified\_model.tar" file

The model source code is written in Fortran 90/95 programming language. There are three makefiles provided. "Makefile" is for a SGI Origin 3800 computer, "Makefile\_snow" is for an Itanium2 cluster and the "Makefile\_njord" is for an IBM power5+ cluster. The run script, "modrun.pl", is written in Perl and is initially meant for an Itanium2 cluster. A detailed description about how to handle this script is given in Chapter 4, "Submitting a Run".

## 1.5 Model grid

The current EMEP model version and the provided input data have a horizontal resolution of  $50 \times 50$  km<sup>2</sup> and are defined on a polar stereographic projection with 20 sigma levels vertically. The model uses the same horizontal and vertical grid resolution as the meteorological data provided with the model. The physical description is given in detail in Chapter 2 of the EMEP Status Report 1/2003 Part I (Simpson *et al.*, 2003).

The technical description of the EMEP model grid is also given on the EMEP website: http://www.emep.int/grid/index.html with details of the projection, and conversion to/from latitude-longitude coordinates.

# Chapter 2 Input files

This chapter provides an overview on the necessary input files to run the Unified EMEP model. A complete set of input files is provided in the EMEP Open Source webpage to allow model runs for the year 2005.

**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.

The standard input files for the Unified EMEP model are provided in two different formats, netCDF or ASCII. The 3 hourly meteorological input data and the initial and boundary conditions data are in netCDF format, and all other input data are in ASCII. Table 2.1 gives an overview over the input files needed for a model run. The first part of the table presents grid dependent netCDF and ASCII files and the last part presents grid independent data. This separation of the files is done for easier overview of input if changes are needed to be done to model resolution and area (grid dependent data). In the downloadable tar file, grid dependent and grid independent input files are distributed in two respective separate subdirectories. The grid dependent data presently provided are at  $50 \times 50$  km<sup>2</sup> resolution covering the EMEP area with  $170 \times 133$  gridpoints. References can be found in Section 1.5.

Please note that some of the ASCII input files contain a header that explains the content of the file. It is desirable that all ASCII input files have such headers, but so far only 6 have this type of header. Work is in progress at EMEP/MSC-W to recode the model version to allow for a full set of input data with header, and will be reported in future releases of the Unified EMEP model code. For the files without a header, the user is recommended to check the actual Fortran module reading the input file for further understanding the formats and usage if description given below is insufficient. Table 2.1: List of input data files. Note: YYYY: year, MM: month, DD: day, SEASON: 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>). ASCII<sup>\*</sup> means ASCII files with header.

Data	Name in the code	Format
Meteorology data directory	$EMEP\_metdata/YYYY/$	
Meteorology	meteoYYYYMMDD.nc (365+1 files)	netCDF
Grid-dependent data directory	$EMEP\_GriddedData/$	
Boundary and initial conditions	Boundary_and_Initial_Conditions.nc	netCDF
Landuse	Inputs.Landuse	$ASCII^*$
BVOC emissions	Inputs.BVOC	$ASCII^*$
Roughness lengths	rough.170	ASCII
Sites locations for surface output	sites.dat	$ASCII^*$
Sondes locations for vertical output	sondes.dat	$ASCII^*$
Snow cover	snowcMM.dat.170 (12 files)	ASCII
Natural $SO_2$	natso2MM.dat.170 (12 files)	ASCII
Volcanoes	Volcanoes.dat	ASCII
Emission data directory	EMEP_GriddedData/Emissions/	
Emissions	GridPOLL (7 files)	ASCII
Grid-independent data directory	Common/	
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	lt21-nox.datMM (12 files)	ASCII
Military aircraft emissions	amilt42-nox.dat	ASCII
Commercial aircraft emissions	aSEASONt42-nox.dat (4 files)	ASCII
VOC speciation	vocsplit.defaults. $BASE\_MAR2004$	ASCII
	$vocsplit.special.BASE\_MAR2004$	ASCII
NO <sub>x</sub> speciation	noxsplit.default.2000	ASCII
	noxsplit.special.BASE_MAR2004	ASCII
Emission factors for scenario runs	femis.dat	ASCII
Photo-dissociation rates	jclear.SEASON (4 files)	ASCII
	jcl1.SEASON (4 files)	ASCII
	jcl3.SEASON (4 files)	ASCII

## 2.1 NetCDF files

The 3-hourly meteorological input data and the boundary and initial conditions input files are provided in netCDF format. We presently follow as much as possible the netCDF CF1.0 conventions (http://www.unidata. ucar.edu/software/netcdf/) for both input and output data (except the Boundary\_and\_Initial\_Conditions file which is still in GDV convention).

## Meteorology

The meteorological input data is from PARLAM-PS - a dedicated version of the HIRLAM (HIgh Resolution Limited Area Model) Numerical Weather Prediction (NWP) model.

The daily "meteoYYYYMMDD.nc" files with 3-hourly values are in netCDF (CF1.0 convention) format.

The parameters extracted from the HIRLAM Meteorological output currently used for Unified EMEP Model runs are given in Table 2.2. A further description of these meteorological fields is given in Chapter 3 of the EMEP Status Report 1/2003 Part I (Simpson *et al.*, 2003).

#### Acknowledgement: met.no

Please acknowledge The Norwegian Meteorological Institute in all publications using these data.

Parameter	Unit	Description
3D fields - for 20 $\sigma$ levels		
u,v	m/s	Wind velocity components
q	kg/kg	Specific humidity
$\dot{\sigma}$	$s^{-1}$	Vertical wind in $\sigma$ coordinates
heta	Κ	Potential temperature
CL	%	Cloud cover
PR	mm	Precipitation
2D fields - for Surface		
Ps	hPa	Surface pressure
T2	Κ	Temperature at 2m height
SH	${\rm W}~{\rm m}^{-2}$	Surface flux of sensible heat
LH	${\rm W}~{\rm m}^{-2}$	Surface flux of latent heat
au	${\rm M}~{\rm m}^{-2}$	Surface stress
SST	Κ	Sea surface temperature
Rh2	%	Relative humidity at 2m height

Table 2.2: Input meteorological	l data	used i	in the	Unified	EMEP	Model
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#### **Boundary and Initial Conditions**

Initial concentrations of major long-lived species are required in order to initialise 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.

Currently one file "Boundary\_and\_Initial\_Conditions.nc" with monthly averaged fields in netCDF (GDV convention) format is needed for Unified EMEP model runs.

This file contains concentrations of CH3COO2, H2O2, OH and O3. The concentrations of CH3COO2, H2O2 and OH are based on previous model runs and were originally intended for use as background concentrations in a simplified version of the Unified EMEP model containing mainly sulphur and nitrogen chemistry. The initial and background concentrations are based on the Logan (1998) climatology. The Logan climatology is scaled 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).

## 2.2 ASCII files

All other input files including the emissions, landuse, timefactors, etc. are in ASCII format.

### Landuse

Landuse data are required for modelling booundary layer processes (i.e. dry depositon, turbulent diffusion). The Unified EMEP model can accept landuse data from any data set covering the whole of the domain and providing reasonable resolution of 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 Centre 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 modelling and effects work.

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

There is a **header** in the file that contains short abbreviations for the different landcover types, e.g. CF for temperate/boreal coniferous forest.

The landuse types are summarised in Table 5.1 in Chapter 5 of the EMEP Status Report 1/2003 Part I (Simpson *et al.*, 2003).

## **BVOC** emissions

Biogenic emissions of isoprene and (if required) monoterpene are calculated in the model as a function of temperature and solar radiation, using the landuse datasets. For more details about how the calculations are performed, please read 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 provided in an **ASCII** file "Inputs.BVOC".

The file contains a **header** and 4 columns. The first two columns are representing the 'i' and 'j' indices of the EMEP grid and the third and fourth columns representing the isoprene and terpene emission potentials with the unit  $\mu g/m^2/h$ .

## Roughness length

The roughness lenght data (which is taken from HIRLAM) are mainly used to assign 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 "rough.170" contains 3 columns. The first two columns represent the 'i' and 'j' indices of the EMEP grid and the third column gives the length with unit: m.

### Sites location for surface output

The model provides a possibility for extra output data of surface parameters (e.g. daily concentrations, meteorology) for selected measurement sites, which will be written to the output files "sites.MMYY".

The **ASCII** file "sites.dat" contains a list of measurement stations for which such output data are wanted. This file can be changed by the users according to their needs.

The input file contains a **header** explaining the 4 columns. The first column is indicating station name, the second and the third columns give the station coordinates ('i' and 'j' indices of the EMEP grid), and finally the fourth column gives the site's vertical coordinate as sigma level (20=ground).

#### Sondes location for vertical output

The model provides a possibility for extra output data of concentration vertical profiles (e.g. daily concentrations, meteorology) for selected measurement sites, which will be written to the output files "sondes.MMYY".

The **ASCII** file "sondes.dat" contains a list of measurement stations for which such output data are wanted. This file can be changed by the users according to their needs.

The input file contains a **header** explaining the 4 columns. The first column is indicating station name, the second and the third columns give the station coordinates ('i' and 'j' indices of the EMEP grid), and finally the fourth column gives the site's vertical coordinate as sigma level (20=ground or surface).

#### Snow cover

Climatological snowcover are provided as monthly gridded **ASCII** files called "snowcMM.dat.170".

The file contain 3 columns; 'i', 'j' indices of the EMEP grid and 'value' in each of the 12 files. The value is either 1 or 0 depending on whether snow is present or absent in the EMEP grid cell at surface.

#### Natural SO2

Natural  $SO_2$  emissions (DMS from sea) are provided as monthly gridded **ASCII** files.

There are 3 columns; 'i', 'j' indices of the EMEP grid and 'value' in each of the 12 files. The values are given with the unit  $\mu g/m^3$  in each EMEP grid cell at surface.

#### Volcanoes

Emissions of 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 "Volcanoes.dat" in **ASCII** format contains only two volcanoes which are the only active volcanoes in Europe. You might notice that "Etna, Italy" appears twice in the input file, which is due to its large base area which shares two grid cells in the model.

The 3 columns give the volcanoes coordinates in the EMEP grid and the volcanoes' height (as sigma level).

#### Emissions

The emission input for the Unified EMEP 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 "gridPOLL" are available in **ASCII** format for the following compounds: CO, NH<sub>3</sub>, NO<sub>x</sub>, PM<sub>2.5</sub>, PM<sub>co</sub>, SO<sub>x</sub> 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 rest 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: *Tonnes*.

Acknowledgement: EMEP

#### Time factors for monthly emissions

Monthly time factors are provided for emissions of the 7 compounds (CO,  $NH_3$ ,  $NO_x$ ,  $PM_{2.5}$ ,  $PM_{co}$ ,  $SO_x$  and VOC).

There is one file "MonthlyFac.POLL" per compound available in **ASCII** format.

There are 14 columns in the monthly files. The first column represents the country code (http://www.emep.int/grid/country\_numbers.txt), the second column represents the sector (http://webdab.emep.int/sectors. html, and then follow the 12 time factors corresponding to months of the year.

Acknowledgement: GENEMIS, IER

## Time factors for daily emissions

Daily time factors are provided for emissions of the 7 compounds (CO,  $NH_3$ ,  $NO_x$ ,  $PM_{2.5}$ ,  $PM_{co}$ ,  $SO_x$  and VOC).

There is one file "DailyFac.POLL" per compound available in **ASCII** format.

There are 9 columns in the daily files. The first column represents the country code (http://www.emep.int/grid/country\_numbers.txt), the

second column represents the sector (http://webdab.emep.int/sectors. html), and then follow the 7 time factors corresponding to days of the week.

Acknowledgement: GENEMIS, IER

#### Landuse definitions

For those vegetative landuse categories for which stomatal modelling is undertaken, the start and end of the growing season (SGS, EGS) with latitude dependent data to capture north-south differences and the development of the leaf area index (LAI) within this growing season must be specified. There is a schematic of LAI development in Figure 5.1 in Chapter 5 of the EMEP Status Report 1/2003 Part I (Simpson *et al.*, 2003).

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

The file contain a **header** explains briefly 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 gives the maximum height of vegetation (m), the fifth indicates albedo (%) and the sixth indicates possible source of NH<sub>x</sub> (0/1). 7 to 10 column is about growing season (day number), 11 and 12 indicates the LAI minimum and maximum  $(m^2/m^2)$  and then 13 and 14 column represent the length of the LAI increase and decline periods (no. of days).

## Stomatal conductance

Parameters for the stomatal conductance model, deposition of  $O_3$  and stomatal exchange (DO3SE) that are based upon the ideas in Emberson *et al.*, 2000, and further discussed in Simpson and Emberson, 2006, must be specified.

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

The file contains a **header** indicating the contents of the file with the different factors needed for each of the landuse classes used in the Unified EMEP model. The first two columns are representing the landuse code (which are consistent with those in "Landuse.Input" file) and name. The next 22 values are different phenology factors.

#### Lightning emissions

Emissions of NO<sub>x</sub> 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".

#### Military aircraft emissions

Annually averaged aircraft emissions are included in the model for  $NO_x$ , (Gardner *et al.*, 1997). The military aircraft emissions are read in as gridded data tabulated on a 128×64 long-lat grid with 12 vertical levels, with global coverage from an **ASCII** file "amilt42-nox.dat".

## Commercial aircraft emissions

Seasonally averaged aircraft emissions are included in the model for  $NO_x$ , (Gardner *et al.*, 1997). Seasonal commercial aircraft emissions are read in as gridded data tabulated on a  $128 \times 64$  long-lat grid with 16 vertical levels, with global coverage.

There are 4 **ASCII** files "aSEASONt42-nox.dat" for each season; January, April, July and October (jan represents winter, apr represents spring, jul represents summer, oct represents autumn).

## **VOC** speciation

Speciation of VOC emissions are specified for each source-sector, derived from the detailed United Kingdom speciation given in PORG (1993). The Unified EMEP model uses a 'lumped-molecule' approach to VOC emissions and modelling, in which for example model species NC4H10 represents all C3+ alkanes, and o-xylene represents all aromatic species. Therefore, each of the species from the detailed UK inventory has been assigned to one of the Unified EMEP model's species according to its reactivity and chemical composition, as given in Andersson-Sköld and Simpson (1997). Although the exact VOC speciation used can be varied ("vocsplit.special.BASE\_MAR2004") to suit particular emission scenarios (e.g. Reis *et al.*, 2000), a default split ("vocsplit.defaults.BASE\_MAR2004") is typically used, as given in Table 4.3 in Chapter 4 of the EMEP Status Report 1/2003 Part I (Simpson *et al.*, 2003).

There are two available **ASCII** files which one can choose to run the model with, depending on whether a particular scenario should be suited

or not. However, the files "vocsplit.defaults.BASE\_MAR2004" and "voc-split.special.BASE\_MAR2004" have currently the same content.

## NO<sub>x</sub> speciation

Speciation of  $NO_x$  emissions are specified for each source-sector and for each country if the file "noxsplit.special.BASE\_MAR2004" is chosen for the model run. The amount of NO<sub>2</sub> compared to other NO is determined by these split-files.

There are two downloadable **ASCII** files which one can choose to run the model with, depending on whether a particular scenario should be suited or not. The file "noxsplit.default.2000" is only sector dependent and the file "noxsplit.special.BASE\_MAR2004" is both sector and country dependent.

## Emission factor for scenario runs

Scenario run in the case of the Unified EMEP 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 10 columns. 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 next 7 columns one can specify which emissions to reduce. Here 1.0 means 100% emissions 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.

### 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; January, April, July and October (jan represents winter, apr represents spring, jul represents summer, oct represents autumn). For light cloud the four seasonal files are called "jcl1.SEASON", for dense cloud conditions the four seasonal files are called "jcl3.SEASON", and then for clear sky the one file is called "jclear.dat".

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).

# Chapter 3 Output files

Output files from a model run are written out in either ASCII, or (for most data outputs) in netCDF format into the working directory. The path to the working directory can be specified in the run script, "modrun.pl". Details of setting the working environment are given in Section 4.1.3.

For a base run, all the outputs will be stored in a subdirectory called "Base" in the default setup under the working directory specified by the user. A list of the output files are given in Table 3.1.

As one can see in Table 3.1, beside the output data files, a successful model run will also result in a few additional files. Most of these contain some kind of information about the model run itself, except for "Remove.sh", which is an executable file. "Remove.sh" will remove the links to the input data from the "Base" directory at the end of a successfully completed run. This means, that the presence of further files (or links to input data files) in "Base" directory indicates a not completed run.

The user has the possibility to choose what kind of the output data will be written out in the different output data files. We will explain how this can be done in the next chapter, in Section 4.1.5.

More details about the output data files are given below. The additional files will not be discussed here in details, as they are less important and very much self explanatory.

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_inst.nc	Gridded instantaneous 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.MMYY	Surface daily values of a selection	ASCII
	of stations and compounds per month.	
Base.sites	All data from "sites.MMYY" files in one file.	ASCII
sondes.MMYY	Vertical daily values of a selection	ASCII
	of stations and compounds per month.	
Base.sondes	All data from "sondes.MMYY" files in one file.	ASCII

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

Additional files	Short description	Format
Base_RunLog	Total emissions of different air	ASCII
	pollutants per country	
eulmod.res	Mass budget of different compounds	ASCII
INPUT.PARA	List of input parameters	ASCII
Remove.sh	Removes the links to the input data at the	ASCII
	end of the run	
Timing.out	Timing log file	ASCII

## 3.1 ASCII outputs: sites and sondes

A model run will produce the following ASCII output files, which can be used for comparison of model results with measurements:

• sites.MMYY and Base.sites

These files contain information on the surface concentrations of different species for a set of specified measurement site locations. These locations are given (and can be modified) in the input file "sites.dat", in which 8 measurement stations in the EMEP domain are listed now.

## • sondes.MMYY and Base.sondes

These files contain information on the concentrations of different species in a vertical column above a set of specified radiosonde locations. These locations are given (and can be modified) in the input file "sondes.dat", in which 27 radiosonde sites in the EMEP domain are listed now.

Both sites and sondes are specified and handled in similar ways in the module **Sites\_ml.f90**. The species and meteorological data required in the output files are defined in **My\_Outputs\_ml.f90**. Furthermore, the time resolution can also be specified in **My\_Outputs\_ml.f90** by the user. (See Section 4.1.5.)

There is a "sites.MMYY" and a "sondes.MMYY" output file for each month of the run period. These monthly outputs are summarized for the whole run period in "Base.sites" and "Base.sondes", respectively.

The outputs start with a header giving the number and the model grid coordinates of the sites used, time resolution, and finally the total number and list of output parameters (species and meteorological data). Below the header the actual values for concentrations are given for each site and each day of the given month (or run period in the case of "Base.sites" and "Base.sondes").

In the "sondes" files values are given for all 20 vertical levels, starting with the ground-level values. On the other hand, "sondes" outputs contain concentrations of fewer species than "sites" output.

The main differences between the structure of "sites.MMYY" ("Base.sites") and "sondes.MMYY" ("Base.sondes") outputs are summarized below:

## Concentration data in sites.MMYY and Base.sites:

• 63 variables (species and meteorological data) are included in the default setup. It can be modified by the user in **My\_Outputs\_ml.f90**.

- Outputs are written out hourly for each day in the present version, but less frequent outputs can be specified in My\_Outputs\_ml.f90.
- Concentration values for only one vertical level are given. For the site locations presently included in "sites.dat", it is the ground level. Other levels can be specified for comparison with, for example, measurements at mountain tops.

## Concentration data in sondes.MMYY and Base.sondes:

- 13 variables (species and meteorological data) are included in the default setup. It can be modified by the user in My\_Outputs\_ml.f90.
- Outputs are printed for hour 0 and 12 for each day in the present version, but more frequent outputs can be specified in My\_Outputs\_ml.f90.
- Concentration values for 20 vertical levels are given, starting with the ground level.

For example, a data block in "sites.0705" (and in "Base.sites") is given as:

20	05 7 6 22	0	
9.338E-03	4.124E+00	8.219E-01	9.298E-03
2.031E-01	2.235E-04	4.954E-02	1.996E-06
4.400E-03	5.940E-03	1.594E-06	4.589E-02
4.804E-02	7.749E-01	8.452E-03	8.180E-01
1.884E+00	1.832E+00	1.507E-01	4.482E-02
5.629E-04	3.216E-02	3.408E-03	6.838E-03
1.586E-04	6.510E-04	6.930E-03	8.935E-04
7.547E-05	4.578E-04	1.188E-03	2.866E-02
1.431E-03	9.397E-05	5.685E-02	1.659E+00
1.332E+02	1.832E+03	4.934E-01	3.305E-01
1.217E+00	6.611E-01	3.849E-41	1.709E-01
1.875E-01	1.639E-01	3.523E-11	1.621E-12
3.341E+02	2.873E+02		
	20 9.338E-03 2.031E-01 4.400E-03 4.804E-02 1.884E+00 5.629E-04 1.586E-04 7.547E-05 1.431E-03 1.332E+02 1.217E+00 1.875E-01 3.341E+02	200576229.338E-034.124E+002.031E-012.235E-044.400E-035.940E-034.804E-027.749E-011.884E+001.832E+005.629E-043.216E-021.586E-046.510E-047.547E-054.578E-041.431E-039.397E-051.332E+021.832E+031.217E+006.611E-011.875E-011.639E-013.341E+022.873E+02	2005762209.338E-034.124E+008.219E-012.031E-012.235E-044.954E-024.400E-035.940E-031.594E-064.804E-027.749E-018.452E-031.884E+001.832E+001.507E-015.629E-043.216E-023.408E-031.586E-046.510E-046.930E-037.547E-054.578E-041.188E-031.431E-039.397E-055.685E-021.332E+021.832E+034.934E-011.217E+006.611E-013.849E-411.875E-011.639E-013.523E-113.341E+022.873E+02

The first line tells us that these are concentration values for the station in Weybourne (UK), the date is 06 July 2005, the time is 22:00. From the second line concentration values for 63 variables are listed. A data block in "sondes.MMYY" and "Base.sondes" files is rather similar to that above. The difference is that here concentration values of each variable are given for each of the 20 vertical levels defined in the model. Thus, in one data block there are (*number\_of\_variables* \* 20) concentration values, e.g. 13 \* 20 = 260 in the default setup.

## **3.2** NetCDF outputs

We follow the netCDF CF1.0 conventions for the netCDF outputs.

The netCDF output files contain gridded 2D and 3D data fields of a selection of species and meteorological variables. The user can self choose from an extensive set of predefined possible output fields those ones, which are needed in the netCFD output files.

Definitions of possible outputs are given in module **Derived\_ml.f90**, and the user can list the wanted fields in **My\_Derived\_ml.f90**. Details of setting the netCDF output are discussed in Section 4.1.5.

The data fields which are written into the netCDF output files from the model runs consist of either 2D or 3D arrays, with some identifiers. Some data fields will contain concentration, others depositions, still others user defined fields.

According to the type of species or meteorological variables the data fields describe, they can contain either averaged or accumulated data. For example, data for precipitation or wet deposition of different chemical compounds need to be accumulated, while concentrations in the air for advected species, e.g.  $NO_2$ ,  $SO_2$  etc., will be averaged. Whether the data for a given compound or variable should be averaged or accumulated, is defined in **Derived\_ml.f90**.

The Unified model attempts to deal with the various possible data fields through a consistent methodology, treating all of the above as simply "derived" fields.

The user has 5 possibilities for choosing the output time periods, namely the outputs can be instantaneous, hourly, daily, monthly and yearly. According to the chosen time period, the data fields are printed in different files, such as:

- **Base\_inst.nc**: instantaneous data output
- **Base\_hour.nc**: hourly data output

- Base\_day.nc: daily data output
- **Base\_month.nc**: monthly data output
- Base\_fullrun.nc: yearly data output

For each possible output field it is defined in **Derived\_ml.f90** whether instantaneous, daily, monthly or yearly data are printed into the netCDF output files. This can be modified by the user taking into account the disk place limitations. More details are given in Section 4.1.5.

The output of hourly data is treated separately from the other output routines in module **Output\_hourly.f90**. Hourly data can be given only for 2D fields and the default output is printed for a smaller domain than the full model domain, because of disk place limitations. We do not recommend to change this.

## Chapter 4

## Submitting a Run

In this chapter we provide detailed information on how to run the regional Unified EMEP model for 3 different types of simulations, namely:

## • Base run

This is the default set up for yearly transport model calculations in  $50x50 \text{ km}^2$  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 sourcereceptor calculations.

## • Tracer simulation

Transport simulations for a single tracer are also possible to perform with the Unified EMEP model.

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.

As explained in the previous chapters, once the model tar file is untarred and all the files are located in the directory called *Unify/Unimod.rv3/*, one can find the run script with name "modrun.pl" in this directory.

"modrun.pl" is a Perl script which governs the compilation of the appropriate "Makefile" and Fortran modules. This script should be submitted for run after the necessary modifications are done with respect to the user's demands. The procedure for running the "modrun.pl" script is somewhat different on different computer systems. In the example given below we assume that we submit a run on a Linux cluster.

## 4.1 Base run

"modrun.pl" allows the user to choose the time period, inputs, work environment etc., without having to change any Fortran files by hand. The script is very much self explanatory, but the most used modification options are also explained in detail below.

The user can also choose outputs and domain of the simulation, but to do so, minor changes in some of the Fortran modules are necessary. Detailed description of how to set user requirements will be given below.

An extract from "modrun.pl" is given in 4.1.7 related to a "Base run" for three months, from January until March, in the year 2005.

## 4.1.1 Setting number of CPUs

The number of CPUs (nodes) requested for the run can be set in the beginning of the run script, "modrun.pl". In the following example we are using 32 CPUs, which is specified (in a PBS queuing system) with the PBS command

## PBS -lnodes=32

If the user changes the number of CPUs in "modrun.pl", it is very important to make modifications in the Fortran file called **ModelConstants\_ml.f90** as well. In this file we define the actual number of CPUs in x-direction (**NPROCX**) and in y-direction (**NPROCY**). The product of these two integer parameters must be equal to the number of CPUs set in "modrun.pl". So, if we require 32 CPUs in "modrun.pl", as in the above example, then we have to set **NPROCX** to 8 and **NPROCY** to 4 in **ModelConstants\_ml.f90**, i.e.

NPROCX = 8 & ! Actual number of processors in longitude
, NPROCY = 4 & ! Actual number of processors in latitude

## 4.1.2 Setting the length of the run

The length of the run can be set in "modrun.pl" using different options. If one wants to run the model for a specific number of months, the run period can be set with

my \$mm1 and my \$mm2,

where the first one defines the first month of the run and the latter sets the last month. The months should be given with two digits, e.g. 04 for April.

In order to submit a few days run from the first day of a given month (defined in **\$mm1**), the number of timesteps, **NTERM**, should be calculated manually as

 $\mathbf{NTERM} = (number\_of\_days) * (terms\_per\_day) + 1,$ 

where  $terms\_per\_day = 8$ .

The number of calculated terms should then be written in **NTERM**. For example, for a run of three days **NTERM=25**(= 3 \* 8 + 1).

## 4.1.3 Setting the work environment

The work environment can be specified in the run script, "modrun.pl". The following directories and paths should be defined:

Username The username should be set with

**my \$MYNAME** = YOURNAME

Input data Please check that all the meteorological and emission data are in place. (See Section 4.1.4 for details.) The main data directory is specified with **\$DataDir**. The path to the meteorological input should be set with **\$MetDir**, and the path to the emission files is given with **\$emisdir**:

my \$DataDir = YOUR\_MAIN\_INPUT\_DATA\_DIRECTORY\_PATH
my \$MetDir = YOUR\_METEOROLOGY\_DATA\_DIRECTORY\_PATH
my \$emisdir = YOUR\_EMISSION\_DATA\_DIRECTORY\_PATH

Model code directory The path to the directory containing the model code is set with **\$ProgDir** :

my **\$ProgDir** = YOUR\_EMEP\_CODE\_DIRECTORY\_PATH

Working (output) directory The working directory where your model output will be written should be specified with **\$WORKDIR**:

**my \$WORKDIR** = YOUR\_WORKING\_DIRECTORY\_PATH

## 4.1.4 Necessary input files

Before submitting a run, please check that all input data files which are required for a model run are downloaded and placed in the proper directories. A summary table of the input files is given in Table 2.1.

Please note the following:

- In order to minimize the necessary changes in the Perl run script "modrun.pl", it is recommended that the structure and naming of the directories containing the grid-dependent data files (*EMEP\_GriddedData/*) and grid-independent data files (*Common/*) is kept as it is.
- It is also advisable to store the meteorological data for a given year in one directory named with the year itself, i.e. meteorology data files for 2005 should be preferably stored in *EMEP\_metdata/2005/*.
- If all input data (sub)directories are accumulated in the same directory, e.g. in *input\_data*, the only input data path to be set in "modrun.pl" is my \$DataDir:
  my \$DataDir = YOUR\_MAIN\_INPUT\_DATA\_DIRECTORY\_PATH
- It is of course fully possible to use different structure and naming, but in that case, please check carefully the list of input files in "modrun.pl" to be sure that the path references are correct.

## 4.1.5 Setting output requirements

The output files from a model run are described in Chapter 3. In this section we will explain how to choose what kind of output data will be printed in the different output data files.

## **ASCII OUTPUTS:** sites and sondes

These files contain information on the concentrations of different species for a set of specified measurement site locations. The "sites" files contain only surface concentration values, while in the "sondes" files concentration values are given for all 20 vertical levels.

The user has the following possibilities for changing the default output:

## • Choosing measurement site or radiosonde location

This can be done by modifying the input files "sites.dat" and "sondes.dat", where the locations are specified. The user can remove sites from these files, or eventually add new ones to it. The list of measurement stations and radiosonde locations from these files are read in by module **Sites\_ml.f90**. The locations are specified for example as:

Weybourne 87 54 20

This refers to a measurement site with name "Weybourne" having x coordinate "87" and y coordinate "54" in the model coordinate system. The last number "20" shows the elevation level, which is in this case the ground level.

Other levels can be useful for comparison of model results with measurements at mountain tops above the model topography.

New sites can be specified in the same way by adding new lines in "sites.dat" and "sondes.dat", but please note that for the present model release, we recommend that the locations are given in 50x50 km<sup>2</sup> model grid coordinates!

### • Choosing output frequency

The user can choose how frequent outputs should be written into the "sites" and "sondes" files. This can be specified in Fortran module **My\_Outputs\_ml.f90** in the following lines:

,FREQ\_SITE = 1 & ! Interval (hrs) between outputs
,FREQ\_SONDE = 12 & ! Interval (hrs) between outputs

The first one sets the time interval given in hours for "sites", while the second one for "sondes" outputs.

## • Choosing species and meteorological data

The species and meteorological data required in the output files are defined in Fortran module **My\_Outputs\_ml.f90**, and can be modified here. For example, for "sondes" outputs we have the following list of species now:

```
integer, public, parameter :: &
  NSONDES_MAX =
                  99
                        & ! Max. no. sondes allowed
 ,NLEVELS_SONDE =
                  20
                        & ! No. of k-levels (9 => 0--2500m)
 ,FREQ_SONDE =
                  12
                        & ! Interval (hrs) between outputs
 ,NADV_SONDE =
                   8
                        & ! Number of advected species
 ,NSHL_SONDE =
                  1
                        & ! No. of short-lived species
 ,NXTRA_SONDE =
                   4
                        &
                           ! No. of Misc. met. params (now th)
                  10
                            ! No. of N species in NOy
 ,N_NOy
integer, public, parameter, dimension(NADV_SONDE) :: &
SONDE_ADV = (/ IXADV_03, IXADV_N02, IXADV_HN03, IXADV_aN03, &
IXADV_pNO3, IXADV_SO4, IXADV_aNH4, IXADV_NH3/)
integer, public, parameter, dimension(N_NOy) :: &
NOy_SPEC = (/ IXADV_HNO3, IXADV_NO, IXADV_NO2, IXADV_PAN,
                                                              &
             IXADV_MPAN, IXADV_NO3, IXADV_N205, IXADV_ISONO3, &
             IXADV_ISNI, IXADV_ISNIR /)
integer, public, parameter, dimension(NSHL_SONDE) :: &
SONDE_SHL = (/ IXSHL_OH /)
character(len=10), public, parameter, dimension(NXTRA_SONDE) :: &
SONDE_XTRA = (/ "NOy", "z_mid", "p_mid", "th " /)
```

The species are identified by names like "IXADV\_NO2". These names are defined in module **Derived\_ml.f90**. While modifying the list of outputs, it is also necessary to set the integer parameters, which declare the number of the given type of species, to correct values.

## NETCDF OUTPUTS

The netCDF output files may contain both 2D and 3D data fields. Module **Derived\_ml.f90** contains an extensive set of predefined outputs.

The user might choose which of these possible data fields should be written into the output files by modifying the module called **My\_Derived\_ml.f90**. The wanted data fields are defined in the following arrays:

- D2\_SR Most of the 2D data fields. Included in a default run.
- **D2\_EXTRA** Further 2D parameters for model evaluation. Included in a default run if it is not a source-receptor calculation.

- WDEP\_WANTED Wet deposition fields. Included in a default run.
- **DDEP\_WANTED** Dry deposition fields. Included in a default run.
- D3\_WANTED 3D data fields. Not included in a default run, but can be included if it is not a source-receptor calculation. We do not recommend 3D data output in the case of source-receptor calculation because of disk place limitations.

Modification of **My\_Derived\_ml.f90** is necessary if we need 3D data fields! While modifying the above arrays, please check the following:

• In My\_Derived\_ml.f90 we define the maximum number of 2D and 3D outputs as:

MAX\_NUM\_DERIV2D = 200 MAX\_NUM\_DERIV3D = 5

These numbers should be modified if the numbers of chosen 2D and 3D output fields exceed them. This might be needed probably only in the case of 3D fields.

• In My\_Derived\_ml.f90 the following if-block is commented out:

```
!if ( .not. SOURCE_RECEPTOR ) then
! call AddArray(D3_WANTED,wanted_deriv3d,NOT_SET_STRING)
!end if
mynum_deriv3d = LenArray(wanted_deriv3d,NOT_SET_STRING)
```

The above if block must be included in order to get 3D output fields! Please remove the exclamation marks if 3D data is wanted.

In **Derived\_ml.f90** the definitions of 2D and 3D data fields include requirements on the output time periods as well. For example, for the wet deposition of sulphur oxides we use:

!code class avg? ind scale rho Inst Yr Mn Day name unit call AddDef( "WDEP ", F, -1, 1.0e6, F , F ,T ,T ,T ,"WDEP\_SOX","mgS/m2")

The name of the field describing wet deposition of  $SO_x$  is WDEP\_SOX. "F" and "T" are shorthands for false and true, respectively. The first "F" (avg?) tells the code that the field will not be averaged, as wet deposition needs to be accumulated. The second "F" (rho) means that the scale is NOT  $\mu$ g. The next four variables stands for the time fields, and here the first "F" (Inst) and the following three "T" (Yr, Mn, Day) show that we want daily, monthly and yearly output, but not output of instantaneous fields.

These definition should not be modified except for eventual changes in the four time fields. The disk place, which are required by the output files can be reduced if the user chooses not to print out unnecessary time fields by setting some of the "T" (true) values to "F" false.

## 4.1.6 Setting the model domain

It is possible to run the model on a smaller domain than the full regional model domain, which is defined by x coordinates ranging from 1 to 170 and y coordinates ranging from 1 to 133.

However, it is strongly recommended that the area specified by the user starts at least 8 grid points from the model domain boundaries, as the meteorological data are not reliable on the boundaries. For European studies the EMEP area can be a good choice, i.e. x coordinate can vary from 36 to 167 and y coordinate can vary from 12 to 122. Outside this area the meteorological data are less reliable.

To set the domain where the model actually runs, one needs only to specify the coordinates of the new domain in **RUNDOMAIN** in the Fortran module called **ModelConstants\_ml.f90**. For example:

x0 x1 y0 y1 RUNDOMAIN = (/ 36, 167, 12, 122 /) ! EMEP domain

tells the model to run in the domain with x coordinates ranging from 36 to 167 and y coordinates from 12 to 122.

The model coordinate system is defined in the meteorological files, and the model coordinates are related to the official EMEP coordinates by:

```
x_{mod} = x_{off} + 35y_{mod} = y_{off} + 11
```

ļ

At present we do not provide support for the use of the EMEP model with alternative grids or resolutions as these are dependent on the availability of meteorological input data.

## 4.1.7 Example script

The example script given below is for a run of 3 months in year 2005 on a Linux cluster with PBS queuing system.

```
_____
#!/usr/local/bin/perl
#Queue system commands start with #PBS (these are not comments!)
# lnodes= number of nodes, ppn=processor per node (max4)
#PBS -lnodes=32
# wall time limit of run
#PBS -lwalltime=01:00:00
# lpmeme=memory to reserve per processor
#PBS -lpmem=200MB
#
#
use 5.6.0; # perl version
use strict;
use warnings;
use File::Copy qw();
my $year = "2005";
                        # Meteorology and emissions year
( my $yy = $year ) = " s/\d\d//; # Gets e.g. 95 from 1995
my SR = 0;
                     #NEW Set to 1 for source-receptor stuff
# iyr_trend:
# :can be set to meteorology year or arbitrary year, say 2050
my $iyr_trend = $year;
$iyr_trend = "2020" if $SR ; # 2020 assumed for SR runs here
# --- User-specific directories (changeable)
               = "Fred"; #-- CHANGE as appropriate!!!, e.g. = "fred";
my $MYNAME
my $USER
               = $MYNAME;
# DataDir = Main general input data directory --- CHANGE as appropriate!!!
my $DataDir = "/home/$USER/input_data";
my $COMMON = "$DataDir/Common"; # Grid-independent data
my $GRID_DATA = "$DataDir/EMEP_GriddedData"; # Grid specific data
```

```
# We define a USER_DATA directory where own-defined files can be kept. Used
# below just for femis.dat so far, bit e.g. sites.dat, sondes.dat can also
# be located here.
my $USER_DATA
                 = "$DataDir/Common";
                                        # Set to common as default.
                 = "$DataDir/EMEP_metdata/$year" ;
my $MetDir
                = "$GRID_DATA/Emissions";
my $emisdir
                                              # Emission directory.
my $METformat="cdf";
                    # For netcdf-style meteorology
#User directories
my $ProgDir = "/home/$USER/Unify/Unimod.$testv";# input of source-code
my $WORKDIR = "/home/$USER/$testv.$year"; # working and result directory
               = (0,31,28,31,30,31,30,31,31,30,31,30,31);
my @month_days
$month_days[2] += leap_year($year);
           "01";
                        # first month, use 2-digits!
my $mm1
         =
my $mm2
         = "03";
                        # last month, use 2-digits!
my $NTERM_CALC = calc_nterm($mm1,$mm2);
my $NTERM =
             $NTERM_CALC; # sets NTERM for whole time-period
# -- or --
#$NTERM = 2;
                  # for testing, simply reset here
# <----- end of normal use section ----->
```

## 4.1.8 Submission of a job

Once the user verified all the details mentioned above and set everything properly, the run script can be submitted as a batch job from the model code directory. On a Linux cluster the command is: **qsub modrun.pl**. Please check the submission routines on the computer system you use! In "modrun.pl" we assume that the MPI parallel job launcher is "scampiexec". This is set in **my \$PRERUN** as: **my \$PRERUN** = "scampiexec";

Please check which MPI parallel job launcher should be used on the system you intend to submit the job to, and set **my \$PRERUN** accordingly. The status of the run can be checked in the job queue (e.g. with **qstat** on a Linux cluster), and once the submitted job is not any more present in the queue, there should be two new files in the model code directory. On a Linux cluster these are the following:

- **modrun.pl.e**<**jobid**> This file with ".e" extension is the error file and a successful completion of the run will result an empty error file.
- modrun.pl.o<jobid> This file with ".o" extension is the object file, or run log file, and it gives all the details about the run including how many CPU hours it has taken, error messages or warnings from the model, etc.

Please note that the name of these log files might be dependent on the computer system!

If the run crashed due to any reason, please check both the error file and the log file, which will lead you to the reason of the crash. After fixing the problem, the job can be submitted again.

## 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, *input\_data/Common/*.

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 is 100% (1.0) emission 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 which is used 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 factor 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.

Once the "femis.dat" file is edited, the run can be submitted as explained in 4.1.8.

## 4.3 Tracer Simulation

The EMEP model is also tested for passive tracer simulations. The code contains the test case of radon  $(^{222}Rn)$  emission from non-ice covered land and water at the rate of 1 atom/cm<sup>2</sup>/s. This is included in the Fortran

module **Setup\_1d\_ml.f90** in the model code. (The user might run a search for "Rn222" in the code.)

Since radon decays into lead (<sup>210</sup>Pb), the emission of <sup>210</sup>Pb is formulated in the code with the decay reaction of <sup>222</sup>Rn. Thus, there are two tracers included in the EMEP code at the moment. Due to the rather longer life time of <sup>210</sup>Pb ( $\sim$ 22 yrs), further decay of this substance is not included. Output variables for the tracers are written out together with other pollutants in the same output file.

This means that in general a "Base Run" includes two passive tracers as well as the other chemical compounds. In order to perform tracer simulation tests with other tracers with a constant emission rate, one simply needs to set those in **Setup\_1d\_ml.f90**. An input file with tracer emissions should be possible to be read into the model in the same way as it is done for other pollutants.

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