Documentation of the chemistry-transport model

Chimere
[version chimere 2014b]

NO₂ surface concentrations with a 1.5km model resolution

- This documentation and the model are freely available at the following internet address:
  
  http://www.lmd.polytechnique.fr/chimere/

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- For questions, send an e-mail to chimere@lmd.polytechnique.fr
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Contents

1 Model overview and last changes 11
  1.1 Short Description of the model ................................................. 11
  1.2 Main characteristics ................................................................. 11
  1.3 The CHIMERE software ................................................................. 13
  1.4 Last changes in this version chimere 2014b .................................... 14
  1.5 About this documentation ............................................................. 14

2 First CHIMERE simulation 17
  2.1 Main sources installation ............................................................. 17
  2.2 The first run tutorial ................................................................. 17
    2.2.1 Download required data and programs .................................... 18
    2.2.2 Simulation configuration ...................................................... 19
  2.3 Main options of chimere.par ....................................................... 20
  2.4 Direct run outputs ................................................................. 25
    2.4.1 The output on screen .......................................................... 25
    2.4.2 The output files ................................................................. 26
  2.5 Post-processing the results ........................................................ 27
  2.6 Some figures to validate your first CHIMERE simulation for the 2009 Test Case .... 28

3 CHIMERE model source code 31
  3.1 CHIMERE general code structure ................................................. 31
  3.2 CHIMERE time integration .......................................................... 33
  3.3 Directories ............................................................................. 34
  3.4 Model Files ............................................................................ 35
    3.4.1 Scripts .................................................................................. 35
    3.4.2 Makefiles ............................................................................. 35
    3.4.3 Meteo interface - 1st stage .................................................... 36
    3.4.4 Source directories ............................................................... 37
    3.4.5 Dynamic files generated at runtime ....................................... 38
  3.5 Routine calls sequence ............................................................... 38
  3.6 Parallelism .................................................................................... 39
    3.6.1 Domains division ................................................................. 39
    3.6.2 Recommendations ............................................................... 41
  3.7 The ‘chimere.nml’ model namelist ............................................... 42
  3.8 How to add a variable in the code? ............................................... 44
    3.8.1 From the master to workers .................................................. 44
    3.8.2 From workers to the master .................................................. 44
    3.8.3 Write variable into outfile .................................................. 45
CONTENTS

4 [domains]: Domains and landuse 47
   4.1 The *domains/domaintlist.nml* file 47
   4.2 Land Use Types, Data, and Interface 48
       4.2.1 Land use interface 50
   4.3 Details on output files 51
       4.3.1 Horizontal domain COORD 51
       4.3.2 Vertical grid VCOORD 51

5 [chemprep]: The chemical preprocessor 53
   5.1 Options available in *chimere.par* 53
   5.2 The first-level script *make-chemistry.sh* 54
   5.3 The second-level scripts 54
   5.4 Manual changes of the mechanism 54
   5.5 Syntax of the REACTIONS file 56
   5.6 Syntax of the PHOTORATES file 57

6 Emissions 59
   6.1 Anthropogenic surface emissions 59
       6.1.1 User’s precompiled emissions 59
       6.1.2 The emiSURF interface 59
   6.2 Biogenic emissions 62
       6.2.1 The biogenic emitted species 62
       6.2.2 Biogenic emission interface 63
   6.3 Mineral dust emissions 63
       6.3.1 Dust emissions over Africa 64
       6.3.2 Dust emissions over Europe 67
       6.3.3 Data used for the mineral dust emissions calculations 69
   6.4 Fire emissions 71

7 Depositions and resuspension 73
   7.1 Dry deposition 73
       7.1.1 For gases: 73
       7.1.2 For aerosols: 74
   7.2 Wet scavenging 75
   7.3 Resuspension of particulate matter 75

8 Initial and boundary conditions 77
   8.1 Chemical boundary conditions 77
       8.1.1 Boundary conditions from global models 77
       8.1.2 Structure of the boundary conditions from global models 79
       8.1.3 Adding new sources of input data 81
       8.1.4 Boundary conditions interface 81
       8.1.5 Internal boundary conditions 82
   8.2 Initial concentrations 82
       8.2.1 Initial concentrations species 82
       8.2.2 Initial concentrations interface 82
9 Meteorology

9.1 Meteorological input data ........................................ 83
9.2 Diagnostics of parameters: ..................................... 85
  9.2.1 Management of additional parameters ...................... 85
  9.2.2 Estimation of the vertical velocity ....................... 86
  9.2.3 Deep convection fluxes .................................. 86
9.3 Transport and mixing .......................................... 89
  9.3.1 Horizontal transport .................................... 89
  9.3.2 Vertical transport ...................................... 90
  9.3.3 Turbulent mixing ..................................... 91

10 Chemistry

10.1 The TWO-STEP time numerical solver ......................... 93
10.2 Gas-phase chemistry .......................................... 94
  10.2.1 Chemical mechanisms (gas phase) ......................... 94
  10.2.2 Species list of the reduced MELCHIOR1 gas-phase chemical mechanism ........................................ 95
  10.2.3 Species list of the reduced MELCHIOR2 gas-phase chemical mechanism ........................................ 104
  10.2.4 Species list of the SAPRC-07-A gas-phase chemical mechanism ........................................ 109
10.3 Aerosol processes ............................................. 117
  10.3.1 Overview .................................................. 117
  10.3.2 Composition and mathematical representation of aerosols ........................................ 118
  10.3.3 Coagulation .............................................. 119
  10.3.4 Absorption ............................................. 119
  10.3.5 Nucleation ............................................. 120
  10.3.6 ISORROPIA ............................................ 120
  10.3.7 Multiphase chemistry .................................. 121
  10.3.8 Secondary organic aerosol chemistry .................... 122
10.4 Impact of clouds ............................................. 124
  10.4.1 Impact on photolysis .................................... 124
  10.4.2 Wet scavenging ........................................ 125
10.5 Radiative transfers and photochemical reaction rates .... 125
  10.5.1 Processes taken into account ............................ 125
  10.5.2 Optical preprocessing using prep_mie .................... 126
  10.5.3 Fast-JX initialisation .................................. 127
  10.5.4 Online calculation of photochemical reaction rates ........................................ 127
  10.5.5 Using the old photorates? ................................ 127

Bibliography .................................................. 127

A References using CHIMERE .................................. 137
  A.1 Reference papers ........................................... 137
  A.2 List of papers ............................................. 137

B History .................................................. 149
  B.1 chimere2008 ............................................... 149
  B.2 V200606 .................................................. 150
    B.2.1 Parallelization ........................................ 150
    B.2.2 Toolbox ............................................... 150
    B.2.3 Scripts ............................................... 150
    B.2.4 makefiles changes .................................. 151
CONTENTS

C Some scripts used in the CHIMERE suite 153
   C.1 The domains/makeCOORDdomains script for horizontal grid definition 153
   C.2 The util/define_geom script for vertical grid definition 154

D How To install NetCDF under GNU/Linux 155
   D.1 Background 155
   D.2 Download 155
   D.3 Configure NetCDF 155
      D.3.1 ifort 156
      D.3.2 g95 156
      D.3.3 pgf90 157
      D.3.4 ifort 64 bit on Intel EMT64 or AMD Opteron 157
      D.3.5 g95 64 bit on Intel EMT64 or AMD Opteron 157
      D.3.6 pgf90 64 bit on Intel EMT64 or AMD Opteron 158
   D.4 Manually Configure CHIMERE 158

E How To install MPI under GNU/Linux 161
   E.1 Background 161
   E.2 LAM/MPI Installation 161
   E.3 Testing 162
   E.4 Uniprocessor users 162
   E.5 Installation from source 163
   E.6 Open MPI installation 163

F Notes on using CHIMERE with LAM MPI 165
   F.1 Specific case of single node environment 165

G Structure of the CHIMERE netCDF files 167
   G.1 EMIS.[domain].[MM].[SPEC].s.nc and EMIS.[domain].[MM].[SPEC].p.nc 167
   G.2 exdomout.nc 168
   G.3 meteo.nc 170
   G.4 AEMISSIONS.nc 172
   G.5 BEMISSIONS.nc 174
   G.6 BOUN_CONCS.nc 175
   G.7 end.nc 175
   G.8 Fire emissions EMIS.[domain].[MM].[SPEC].f.nc 180
### List of Figures

1.1 General principle of a chemistry-transport model such as CHIMERE. In the box 'Meteorology', $u_*$ stands for the friction velocity, $Q_0$ the surface sensible heat flux, $L$ the Monin-Obukhov length and BLH the boundary layer height. $c_{\text{mod}}$ and $c_{\text{obs}}$ are for the chemical concentrations fields for the model and the observations, respectively. .................................................. 13

2.1 Figures to validate the March 2009 Test Case simulation .................................................. 29

3.1 General structure of CHIMERE model ................................................................. 32

3.2 General CHIMERE structure for time integration of all processes ................................. 33

3.3 Calculation of the number of integration steps per hour to respect the CFL over a complete 120 hours simulation. ................................................................. 34

3.4 Detailed list of CHIMERE routines and time loops ..................................................... 39

3.5 Time processing in CHIMERE ................................................................. 40

4.1 Examples of horizontal domains. The dots represent the MM5 EUR1 grid cells centers and the rectangle represents the boundaries of the CHIMERE CONT3 domain. .................................................. 48

6.1 Top-down processing of EMEP anthropogenic emissions with the emiSURF interface ........ 61

6.2 Domains of mineral dust emissions estimations. ..................................................... 64

6.3 Estimation of weights as a function of the prescribed binding energies $e_1$, $e_2$ and $e_3$. 67

6.4 Relative part of the most important soil class for each model cell. A value of 0.5 means that the most present soil represents 50% of the model cell. .................................................. 69

8.1 Surface ozone concentrations modelled with LMDz-INCA and MACC for july. ................. 79

8.2 Surface mineral dust concentrations modelled with GOCART and LMDzINCA for july. 80

9.1 Flow chart of the meteorological CHIMERE pre-processor. WRF model is shown as an example of a weather forecast model driving CHIMERE. Programs are shown in yellow and NetCDF files in blue. .................................................. 83

9.2 [left] Temperatures changes due to shallow and deep convection and [right] Schematic view of a convective cloud ................................................................. 87

9.3 Entrainment and detrainment fluxes in the updrafts and downdrafts. ................................. 88

9.4 Convective atmospheric column and its environment .................................................. 89

10.1 Principle of ‘operator-splitting’ versus Chimere integration ......................................... 93

10.2 Routines, files and scripts involved in the calculation of radiative transfers ................. 126
## List of Tables

1.1 Main properties of the CHIMERE model ................................................. 12
2.1 Useful URL addresses for the development and the use of the CHIMERE model and its modules ................................. 18
2.2 Variables in the METEO output file. ..................................................... 27
4.1 Landuse categories used in CHIMERE .................................................... 49
4.2 GLCF land cover types used in CHIMERE .............................................. 49
4.3 GlobCover land cover types used in CHIMERE ....................................... 50
6.1 Gas and particle emissions required for MELCHIOR and SAPRC .................. 60
6.2 Notations used to describe the saltation and sandblasting processes. * i=3 in this case. ........................................... 65
6.3 Fractions (p_i) of the kinetic energy for the three binding energies e_i, after [Alfaro et al., 1997] ...................................... 66
6.4 Needed parameters for the mineral dust emissions fluxes calculations ............... 69
6.5 Description of soil types. CS= Coarse sand; FMS=Fine medium sand. .......... 70
9.1 Mandatory and optional variables in exdomout.nc meteo file. Note that all meteorological 3D variables must be provided at half-layers levels. ....................................................... 84
9.2 Constant values used for the calculation of additional parameters in the routine calc_turb. .................................................. 86
10.4 List of aerosol species. (*): ions, molecules, crystals ................................ 118
10.5 Characteristics of the look-up table used for the calculation of the thermodynamic equilibrium with ISORROPIA ................................................................ 121
10.6 Relative humidity at deliquescent points for the species used by ISORROPIA in the system sulfate-nitrate-ammonium-water. ................................ 121
10.7 Gas phase chemical scheme for SOA formation in CHIMERE. The surrogate SOA compounds consist of six hydrophilic species that include an anthropogenic nondissociative species (AnA0D), an anthropogenic once-dissociative species (AnA1D), an anthropogenic twice-dissociative species (AnA2D), a biogenic non dissociative species (BiA0D), a biogenic once-dissociative species (BiA1D) and a biogenic twice-dissociative species (BiA2D), three hydrophobic species that include an anthropogenic species with moderate saturation vapor pressure (AnBmP), an anthropogenic species with low saturation vapor pressure (AnBIP) and a biogenic species with moderate saturation vapor pressure (BiBmP), and two surrogate compounds for the isoprene oxidation products. ........................................... 123
Acknowledgments

The model is developed at IPSL/LMD (Palaiseau), INERIS (Verneuil en Halatte) and IPSL/LISA (Creteil) in France.

For questions about the model development, parameterizations or variables choices, you can send an e-mail to the developers: chimere@lmd.polytechnique.fr.

This will send an e-mail to: Laurent Menut, Dmitry Khvorostyanov, Myrto Valari, Solene Turquety, Sylvain Mailler (LMD), Bertrand Bessagnet, Augustin Colette (INGERIS) and Guillaume Siour (LISA).

For questions about the model use, to share pre- or post-processing tools with the other users, or just present your result, you can register to the chimere users mailing list here: http://www.lmd.polytechnique.fr/chimere/subscribe.php

In case of use of the MACC global dataset as boundary conditions, please add in your publications the following acknowledgment: “This data set was provided by the MACC-II project, which is funded through the European Union Framework 7 programme. It is based on the MACC-II reanalysis for atmospheric composition; full access to and more information about this data can be obtained through the MACC-II web site (http://www.copernicus-atmosphere.eu).”

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Chapter 1

Model overview and last changes

1.1 Short Description of the model

The CHIMERE multi-scale model is primarily designed to produce daily forecasts of ozone, aerosols and other pollutants and make long-term simulations for emission control scenarios. CHIMERE runs over a range of spatial scales from the regional scale (several thousand kilometers) to the urban scale (100-200 Km) with resolutions from 1-2 Km to 100 Km. On CHIMERE server, documentation and source codes are proposed for the complete multi-scale model. However most data are valid only for Europe and should be revisited for applications on other continents.

CHIMERE proposes many different options for simulations which make it also a powerful research tool for testing parameterizations, hypotheses. Its use is relatively simple so long as input data is correctly provided. It can run with several vertical resolutions, and with a wide range of complexity. It can run with several chemical mechanisms, simplified or more complete, with or without aerosols.

Currently, the model may be used for:

- Physical and chemical processes research
  - Transport and mixing, turbulence
  - Aerosols chemistry
  - Dust and fire emissions and transport
  - Particles deposition
  - Clouds, radiation and chemistry
  - Vegetation and chemistry interactions
- Scenarios and climatologies
  - Past and future emissions impacts
  - Ensemble analysis
- Forecast
  - Experimental forecast at LMD
  - Operational forecasts (PREVAIR, AQ networks, GEMS, MACC, etc.)

The main properties of the CHIMERE processes calculations are described in Table 1.1.

1.2 Main characteristics

CHIMERE is an Eulerian off-line chemistry-transport model (CTM). External forcings are required to run a simulation: meteorological fields, primary pollutant emissions, chemical boundary conditions. Using these input data, CHIMERE calculates and provides the atmospheric concentrations of tens of gas-phase and aerosol species over
Table 1.1: Main properties of the CHIMERE model

<table>
<thead>
<tr>
<th>Process</th>
<th>Methodology</th>
</tr>
</thead>
<tbody>
<tr>
<td>Meteorological forcing</td>
<td>ECMWF, GFS, MM5, WRF</td>
</tr>
<tr>
<td>Landuse</td>
<td>GLCF or GlobCover global datasets</td>
</tr>
<tr>
<td>Horizontal resolution</td>
<td>from 1km to few degrees</td>
</tr>
<tr>
<td>Horizontal advection</td>
<td>upwind, Van Leer or PPM</td>
</tr>
<tr>
<td>Vertical advection</td>
<td>upwind or Van Leer</td>
</tr>
<tr>
<td>Deep convection</td>
<td>the Tiedke scheme</td>
</tr>
<tr>
<td>Boundary-layer turbulence</td>
<td>the Troen and Mahrt scheme</td>
</tr>
<tr>
<td>Anthropogenic emissions</td>
<td>EMEP, HTAP or local inventories</td>
</tr>
<tr>
<td>Biogenic emissions</td>
<td>online MEGAN model</td>
</tr>
<tr>
<td>Sea salt emissions</td>
<td>Monahan scheme</td>
</tr>
<tr>
<td>Mineral dust emissions</td>
<td>Alfaro and Gomes scheme</td>
</tr>
<tr>
<td>Chemical mechanism</td>
<td>SAPRC or MELCHIOR</td>
</tr>
<tr>
<td>Aerosols representations</td>
<td>bins</td>
</tr>
<tr>
<td>Secondary Organic Aerosols</td>
<td>Pun scheme</td>
</tr>
<tr>
<td>Photolytic rates</td>
<td>online FastJX radiative transfer model</td>
</tr>
<tr>
<td>Numerical solver</td>
<td>the TwoStep solver</td>
</tr>
<tr>
<td>Aerosol thermodynamic equilibrium</td>
<td>online ISOROPIA</td>
</tr>
<tr>
<td>Dry deposition</td>
<td>Wesely parametrization</td>
</tr>
</tbody>
</table>

local to continental domains (from 1 km to 1 degree resolution). The key processes affecting the chemical concentrations represented in CHIMERE are: emissions, transport (advection and mixing), chemistry and deposition, as presented in Figure 1.1. Note that forcings have to be on the same grid and time step as the CTM simulation. In this sense, CHIMERE is not only a chemical model but a suite of numerous pre-processing programs able to prepare the simulation. The model is now used for pollution event analysis, scenario studies, operational forecast and more recently for impact studies of pollution on health ([Valari and Menut, 2010]) and vegetation ([Anav et al., 2011]).

The first model version was released in 1997 and was a box model covering the Paris area including only gas-phase chemistry ([Honoré and Vautard, 2000], [Vautard et al., 2001]). In 1998, the model is implemented for its first forecast version (Pollux) during the ESQUIF experiment ([Menut et al., 2000b]) still over the Paris area ([Vautard et al., 2000]). At the same time, the adjoint model was developed to estimate the sensitivity of concentrations to all parameters ([Menut et al., 2000a]). In 2001, the geographical domain was extended over Europe with a cartesian mesh ([Schmidt et al., 2001]) and the new experimental forecast platform (PIONEER) is set up. In 2003, the experimental forecast became operational with the PREVAIR system operated at INERIS ([Honoré et al., 2008], [Rouil et al., 2009]). The aerosol module is implemented in 2004 ([Bessagnet et al., 2004]) with further improvements concerning the dust natural emissions and resuspension over Europe ([Vautard et al., 2005a], [Hodzic et al., 2006a] [Bessagnet et al., 2008]) and evaluated against long-term and field measurements ([Hodzic et al., 2005], [Hodzic et al., 2006b]). The development of the mineral dust version started in 2005 ([Menut et al., 2005]). Chemistry was not included in that version and a new horizontal domain had been designed to cover the whole northern Atlantic and Europe, including the Saharan desert and downwind regions. In 2006, an important step is achieved with the development of the parallel version of the model and its first implementation on a massively parallel computer (the ECMWF computer in the framework of the FP6/GEMS project).

The CHIMERE model is now considered as a state-of-the-art model. It has been involved in numerous intercomparison studies mainly focusing on ozone and PM\textsubscript{10} from the urban scale ([Vautard et al., 2007, Van Loon et al., 2007, Schaap et al., 2007]) to continental scale ([Solazzo et al., 2012], [Zyryanov et al., 2012]). Moreover, the model has been mainly applied over Europe, but also more recently over Africa and the North Atlantic for dust sim-
Figure 1.1: General principle of a chemistry-transport model such as CHIMERE. In the box 'Meteorology', $u_*$ stands for the friction velocity, $Q_0$ the surface sensible heat flux, $L$ the Monin-Obukhov length and BLH the boundary layer height. $c_{\text{mod}}$ and $c_{\text{obs}}$ are for the chemical concentrations fields for the model and the observations, respectively.

ulations, over Central America during the MILAGRO project to study organic aerosols ([Hodzic et al., 2009], [Hodzic et al., 2010b], [Hodzic et al., 2010a]) and over the US within the AQMEII project ([Solazzo et al., 2012]). Finally, the development of CHIMERE follows three main rules. First, concentrations of main pollutants are calculated with the best possible accuracy using well evaluated and state-of-the-art parameterisations. Second, a modular framework is maintained to allow updates to the code by developers but also all interested users. Third, the code is kept computationally efficient to allow long-term simulations, climatological studies and operational forecast.

1.3 The CHIMERE software

In order to facilitate software distribution, CHIMERE is protected under the General Public License. The source code and the associated documentation is available on a web site www.lmd.polytechnique.fr/chimere. The documentation is both technical and scientific. It includes a chapter dedicated to the set-up of a test case simulation that allows new users to easily carry out a CHIMERE simulation: model configuration and data (meteorology and emissions files) are provided to simulate the 2003 heat wave in western Europe.

CHIMERE is a National Tool of the French Institut des Sciences de l’Univers, meaning that support has to be provided to the users of model. Two mailing lists exist for this support: chimere@lmd.polytechnique.fr to send questions to the model developers and chimere-users@lmd.polytechnique.fr to initiate discussions, exchange programs or data between users. In addition, two-day training courses are organised twice a year. Each training course is free of charge for participants and offers a complete training to be able to install the code, launch a simulation and change surface emissions or other parameters in the code.

The code is completely written in Fortran90, and running scripts are written in shell (using gnu-awk for input datafiles processing). The required software is a Fortran 95 compiler (g95 and gfortran are both free and efficient, but Makefiles with Intel’s ifort compiler options are also provided). The required libraries are NetCDF (either 3.6.x or 4.x.x), MPI (see below), and GRIB API (associated to the use of the ECMWF meteorological datasets).
model includes tools that can help the user to configure the model’s Makefiles for the libraries already installed. The model computation time for one AMDx64 node of 16 CPUs is 1h30min for 1 month of simulation for the Paris area, at 15 km resolution, the domain size being 45x48x8 with a time step of 360 seconds on average. CHIMERE uses the distributed memory scheme, and MPI message passing library. It is maintained for Open MPI (recommended) and LAM/MPI, but works, with minor changes in the scripts, with MPICH or other MPI compatible parallel environments. The model parallelism results from a Cartesian division of the main geographical domain into several sub-domains, each one being processed by a worker process. Each worker performs the model integration in its geographical sub-domain as well as boundary condition exchanges with its neighbours. In addition a master process performs initialisations and file input/output. To configure the parallel sub-domains, the user has to specify two parameters in the model parameter file: the number of sub-domains for the zonal and meridional directions. The total number of CPUs used is therefore the product of these two numbers, plus one CPU for the master process.

For graphical postprocessing, simple interfaces are available using either the GMT 5 or the GrADS 6 free software. Also an additional graphical user interface (GUI) software CHIMPLOT is provided. It allows making various 1D or 2D plots (e.g., longitude-latitude or time-altitude maps, vertical slices, time series, vertical profiles). One can also overlay multiple fields (e.g., O\textsubscript{3} concentrations, wind vectors, and pressure contours) and perform simple operations such as calculating daily maxima, daily means, vertical or horizontal averaging or integrations.

### 1.4 Last changes in this version chimere 2014b

Version chimere 2014b contains the following improvements:

- **Processes**
  - Added the FastJ radiative transfer model to compute photolysis reaction rates. This makes it possible to extend the model domain vertically beyond 500 hPa. An automatic calculation of optical depth (for clouds and aerosols) is also done.
  - Added possible read of fires emissions fluxes (if provided by the user)
  - Added SAPRC-07-A chemical mechanism
  - Updated ISOROPIA V2006

- **Numerics/Software**
  - Activated adaptive CFL condition. This speeds up computations.
  - Improved deep convection calculation. This speeds up computations and yields more realistic ozone land-sea interfaces.
  - diagmet, diagbio, and diagdust programs are put in the model core.
  - Improved calculations of boundary conditions (with new datasets built with LMDz-INCA, GOCART and MACC global climatologies)
  - Optimized calculations of vertical levels

### 1.5 About this documentation

This documentation describes the last version of the CHIMERE chemistry-transport model named chimere 2014b. The model and associated source codes are freely available on a web site:

http://www.lmd.polytechnique.fr/chimere/

In this documentation:

- Chapter 2 explains how to install the model from scratch and perform a first run using the prepared test case 'Heat Wave summer 2003 over Europe'.
⋄ Chapter 3 (p.31) presents the model sources documentation including the pre- and post-processing interfaces.
⋄ Chapter 4 (p.47) and 5 (p.53), explain how the user may define its own model geometry (domain and landuse) and its own configuration for chemistry (gas and/or aerosols, tracers etc.)
⋄ Chapters 6 (p.59), 8 (p.77), 9 (p.83), 10 (p.93) describe the treatment (processes and numerics) of the emissions, boundary conditions, meteorology and chemistry.
⋄ Appendix presents "how-to" files explaining the way to install libraries such as netCDF and LAM/MPI, and the format of all files used by the model.
⋄ A list of published papers about studies using CHIMERE is displayed in chapter A, p.137.

For further questions, please send an e-mail to the developers at chimere@lmd.polytechnique.fr.
Chapter 2

First CHIMERE simulation

In the case of a user who never used the CHIMERE model before, this chapter presents how to:

- Install all softwares prerequisites, §2.1
- Perform a simulation with the pre-defined test case available on the CHIMERE web site, §2.2, with a complete description of the model top-calling script, §2.3
- See the results, §2.4, post-process the concentrations fields §2.5.

2.1 Main sources installation

The CHIMERE model has only been tested on GNU/Linux systems with LAM-MPI and Open MPI message passing libraries. However it should be working on most UNIX systems provided the following software is installed.

The foreseenable changes should be related to shell, awk and make syntax, to the MPI library used, and also to unformatted binary files which may have to be converted.

The model requires:

- a Fortran 95 compiler (e.g., gfortran)
- GNU bash Bourne shell, awk and make
- Unidata NetCDF library (free)
- Open MPI (http://www.open-mpi.org) or LAM-MPI (Indiana University) software (free)
- The NCO libraries (free)

The installation process of NetCDF and MPI is fully described in §D, p.155 and §E, p.161. The NetCDF library must be compiled with the same compiler as CHIMERE model.

If no bash is installed, the model may work with a baseline Bourne-shell, but the user may have to edit the scripts to take in account some syntactic features specific to bash. The same remark apply to the awk and make utilities. The model has been tested with the following compilers: gfortran, g95, ifort and pgf90.

In the following examples, the wget utility is used for downloading, because it is a robust and powerful downloading tool. However, if wget is not installed on your system, you can obviously use your favorite browser to download files.

The Table 2.1 reports useful URL adresses for the development and the use of the CHIMERE model and its modules.

2.2 The first run tutorial

For the first CHIMERE run, we propose to simulate the particulate matter pollution event occurred over Northern Europe in March 2009.
This Test Case simulation is over the European domain called \textit{CONT5} (defined in \texttt{domains/domainlist.nml}, see below) and lasts 8 days starting from March 12 2009. The PM pollution event occurs on March 19 with a maximum at 14h. To drive CHIMERE, WRF model meteorological fields have been prepared. The WRF simulation was driven by the 6-hourly NCEP/A VN analyses with the spectral "nudging" option (grid FDDA). You can see the detailed list of WRF simulation parameters in the output file \texttt{wrfout*}. The model domain covers the Western Europe with a horizontal resolution of 45km and 30 vertical levels.

### 2.2.1 Download required data and programs

To perform this test case, you need to download the model and some input data archives. To access the source files and databases for the first time, you need to register by filling out the form in the downloads section of the CHIMERE web site: [http://www.lmd.polytechnique.fr/chimere/download.php](http://www.lmd.polytechnique.fr/chimere/download.php). Your data will be examined and if approved you will receive your login/password to access the download page. The script \texttt{chimere-download.sh} is provided to simplify CHIMERE installation. You need to download the script from the web site and to launch it from the directory where you wish to install Chimere. The script does the following:

1. Prompts you to specify the directory where you would like to store large data files. Creates the model directory and subdirectories for the big files, emissions, output, and the meteorology
2. Downloads the CHIMERE source code and data for the test case: EMEP emissions\footnote{For the use of these emissions data, please acknowledge EMEP (Yearly totals), IER (Time variations), TNO (Aerosol emissions), UK Dept of Environment (VOC speciation, Passant, 2002).} preprocessed for July and August and MM5 meteorological output for the 5 days of test simulation.
3. Downloads emission data for other months and the complete emiSURF preprocessor
4.Downloads the boundary and initial conditions
5. Decompresses the downloaded archives to the appropriate directories
6. Moves the archives to the ARCH directory
2.2.2 Simulation configuration

Once the code is downloaded and the mandatory libraries NetCDF and MPI are installed, the next step is to configure CHIMERE for your system.

CHIMERE uses configuration files that reflect user’s requirements and environment. These files reside in chimere 2014b top directory:

- **[Makefile.hdr]** is a symbolic link to a preformated file, specific to a given compiler. It contains all the informations pertinent to your execution environment: compiler options, libraries, and so on. Makefile.hdr is included by all subsequent makefiles in CHIMERE source tree, to ensure a consistent compilation.

- **[mychimere.sh]** contains PATHs to the system software used by CHIMERE: NetCDF and MPI libraries, Fortran compiler, the Makefile.hdr version to use, and the compilation mode (debugging or performance, see below). This file simplifies model portability between different computers, system library versions and Fortran compilers. Once you generated a version of mychimere.sh for a particular system/compiler, you can easily change between them just by changing the symbolic link mychimere.sh to mychimere.sh.[software_version].

- **[chimere.par]** is an ASCII file that unites by topic all main parameters of CHIMERE simulations, such as data file locations, domain definitions, physical and numerical options. It also accepts comments (started with '#'), valid bash commands like
  
  $$\text{date -u -d "${di} ${ndays} days" +%Y-%m-%d}$$

  and supports simplified date arithmetic, e.g.,

  $$((\text{di} - 1))$$

  instead of

  $$\text{date -u -d "$\text{di} 1 days ago" +%Y-%m-%d}$$

  A copy of this file is given in the §2.3, p.20.

To configure CHIMERE:

- Run `config.sh`. 
  
  ```
  ./config.sh mychimere.sh.gfortran_MyLinuxCluster
  ```

  This will generate a version of mychimere.sh corresponding to
  
  ◦ location of your Fortran compiler
  ◦ location of your NetCDF package
  ◦ location of your MPI library and executables
  ◦ if needed, location of your gribex library (for interfaces to meteorologcal datasets in the grib format)

  It will also create a symbolic link mychimere.sh to the newly generated version of the file. Later, during CHIMERE compilation with the compile script and when running the top-calling script chimere.sh, an appropriate symbolic link Makefile.hdr will be created. You can then manually edit mychimere.sh to specify the compilation mode: DEVEL for debugging or PROD for performance.

- Edit chimere.par to:
  
  ◦ set up the time span of a run
  ◦ set the cartesian division of the domain (nzdoms and nmdoms)
  ◦ tell CHIMERE the location of pertinent files and directories including the input data that you downloaded:
    ◦ domain geometry
    ◦ species list
The current Chimere version has been tested with Open MPI. The latter does not need to be booted, you can just launch mpirun with your executable. If you are still using LAM MPI, see p. 165.

- Compile all programs:

```
make clean
./compile - this should be used instead of make, since it sources the current mychimere.sh making the parameters defined there visible to the system during model compilation and linking.
```

Then you can execute the top-calling script chimere.sh. For instance for the proposed test case:

```
chimere.sh
```

and see the messages on the screen to check if installation was correctly done.

### 2.3 Main options of chimere.par

Notes to the top-calling script chimere.sh and the parameter file chimere.par:

- The first optional argument of the script chimere.sh is the starting date. For example, for the tutorial test case, the user could launch the script using chimere.sh 20090312. The parameter ’di’ would have the value ’20090312’ in this case. The starting date ’di’ can be also specified in chimere.par for each of nested simulations. If the ’di’ parameter is specified as the argument of chimere.sh it has a priority over those given in chimere.par.
- Most of the parameters visible to CHIMERE are specified in chimere.par in the format

```
[\$parameter_name] This parameter description : Value1, Val2,.. ValN
```

All parameters initialized this way will be visible to the scripts of CHIMERE during simulations.
- Simulation parameters, such as lab, nested, dom, etc., are given as comma-separated values after the colon character (":") in chimere.par. Each column of values corresponds to a different simulation. The user can run multiple simulations with a single call to chimere.sh. The script will subsequently run simulations with parameters defined by the columns whose numbers are listed in the "RUNS" line in the beginning of chimere.par. This is useful when running nested simulations: e.g., the first column corresponds to a coarse domain, while the second one specifies the fine domain. If for some parameter the number of comma-separated values is less than the number of the simulation requested, the last comma-separated value will be used for that simulation. For instance, you would typically save concentrations to the restart file end....nc at the same frequency for all your simulations, thus having only one value of the $nsconcs parameter.
- Analysis or forecast mode? ($forecast = 0 or 1) If simulation timing parameters (di, de, dib, deb, dim, dem, dibm, debm) are set to 0 in chimere.par, they will be automatically redefined in scripts/check-dates.sh according to the value of the $forecast parameter.
  - In the analysis mode ($forecast = 0), the run duration is ’ndays’, from ’di’ to ’di’+’ndays’-1. If a previous simulation is used to force the current one (with initial conditions), it is assumed to have the same duration ’ndays’ and to span from ’di’-’ndays’ to ’di’-1.
  - In the forecast mode ($forecast = 1), ’ndays’ refers to the maximum forecast time, and the whole simulation period is from ’di’ to ’di’+’ndays’, i.e., ’ndays’+1. The previous simulation used to force the current one spans from ’di’-1 to ’di’+’ndays’-1.
  - Typical ’ndays’ value is 5 days for an analysis run and 4 days for a forecast simulation.
Compilation and execution flags. The user specifies whether to run various CHIMERE components using the following flags:

<table>
<thead>
<tr>
<th>Flag</th>
<th>Action</th>
<th>Script in the <code>scripts/</code> directory</th>
<th>Chimere component(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>imakecompil</td>
<td>Model compilation</td>
<td>chimere-compil.sh</td>
<td>interf-&lt;meteo&gt; and chimere.e</td>
</tr>
<tr>
<td>imakemeteo</td>
<td>Meteorological interface</td>
<td>chimere-meteo.sh</td>
<td>prepmeteo.e</td>
</tr>
<tr>
<td>imakeaemis</td>
<td>Anthropogenic emissions</td>
<td>chimere-aemis.sh</td>
<td>chimere-aemis.sh</td>
</tr>
<tr>
<td>imakedust</td>
<td>Dust emissions</td>
<td>chimere-run.sh</td>
<td>chimere.e</td>
</tr>
<tr>
<td>imakefemis</td>
<td>Fire emissions</td>
<td>chimere-aemis.sh</td>
<td>prepmeteo.e</td>
</tr>
<tr>
<td>iusebound</td>
<td>Initial and boundary conditions</td>
<td>chimere-bound.sh</td>
<td>prep_bc.e/prep_chimere.e</td>
</tr>
<tr>
<td>imakerun</td>
<td>Running Chimere</td>
<td>chimere-run.sh</td>
<td>chimere.e</td>
</tr>
</tbody>
</table>

These flags can be either 1 or 0 meaning to launch or not the corresponding pre-processor. Besides, most of the flags can also have the value of 2. In this case the pre-processor will be launched only if its output file is required and does not already exist. These output files and directories are also specified in `chimere.par`.

The directory specified by the `$datadir` parameter can be used to store dynamic pre-processor files ($exdomout, $fnemisa, $fnemisb, etc.).

The $iusebemis and $iusedust flags determine whether the simulation needs biogenic emissions and dust species, respectively. The $imakedust flag determines whether to generate dust emissions in the model core (chimere.e). Note that $iusebemis and $iusedust flags along with the $imakerun flag use the same model component (chimere.e). They are related to different parts of the code and are independent. For instance, setting $iusedust to 1 and $imakerun to 0 will launch `chimere-run.sh` and chimere.e, so that dust emissions will be computed, but not the model time integration loop.

Here is the listing of the parameter file `chimere.par`:

```bash
# CHIMERE Modeling System Configuration file
# For model code & data downloads, updates, news, and documentation
# see http://www.lmd.polytechnique.fr/chimere
# => The variables mentioned here with the '\$' sign (e.g., $dom) can be further used in expressions
# - given they have been defined BEFORE they are used! Otherwise -> empty string instead!
# => For dates arithmetic, you can use expressions like (($di + 1)) or (($deb - 1)).
#    They will be replaced by valid bash "date" commands with the %Y%m%d format
# => Valid bash commands can also be used, e.g., $(date -u -d "$(di) $ndays days" +%Y-%m-%d)
# => $(${chimere_root}) is where your source chimere files are
# List the simulations to run separated by whitespace in the next line:
#---------------------------------------------
# List the simulations to run separated by whitespace in the next line:
#---------------------------------------------
# Date/Time management
${forecast[Forecast(1) or analysis(0) run]} : 0
${di[CHIMERE run Start Date]} : 20090312 # Overridden by chimere.sh
${ndays[CHIMERE run Duration (0 = auto)]} : 8
${de[CHIMERE run End Date (0 = auto)]} : 0
${dib[CHIMERE prev. run Start Date (0 = auto)]} : 0
${deb[CHIMERE previous run End Date (0 = auto)]} : 0
${dim[Meteo driver Start Date (0 = auto)]} : (($di - 1))
${dem[Meteo driver End Date (0 = auto)]} : (($de + 1))
```

Chimere
# CHIMERE Simulation Domain

- Nested run? (yes/no): no, yes
- CHIMERE domain: CONT5, IDF15C
- Number of parallel zonal subdomains: 5
- Number of parallel merid subdomains: 3
- Number of vertical layers: 8
- Top layer pressure (mbar): 500
- First layer pressure (sigma * 1e3): 997

# Meteorology Driver

- On-line [1] or off-line [0] modeling: 0
- Meteo driver (WRF, MM5, ecm): WRF
- Meteo driver domain: d01, d02

# Simulation Output Files

- Simulation label: Test, TestNest
- Coarse domain label: none, Test
- Number of layers in output file: 8
- Output species detailed (low/full): low
- Cumulated deposition, file dep...: 12
- Current run label (output files’ ending): ${di}_${de}_${lab}
- Label of the run to use its data: ${di}_${de}
- Previous run label: ${dib}_${deb}_${lab}

# Emissions

- Anthropogenic emission source: emep, emep
- Use surface emissions? (1/0): 1, 1
- Use point emissions? (1/0): 0
- Use fire emissions? (1/0): 0
- Need biogenic emissions? (1/0): 1
- Africa: dust by wind erosion? (1/0): 1
- Europe: dust by wind erosion? (1/0): 0
- u* threshold estimation: 1
- Saltation/sandblasting scheme: 2

# Boundary conditions

- Use and build Initial & Boundary conditions?: 1 # 0 – do not use; 1 – use and build; 2 – check if files exist and use

# Chemistry Options

- Chemistry mechanism (0..3): 2, 2
- Chemically-active aerosols (1/0): 1
- Number of aerosol size sections: 10
- Include sea salts? (1/0): 1
- Include POPs? (1/0): 0
- Include carboneceous species?: 1
- Include dust species and emissions? (1/0): 1
- Secondary organic aerosol scheme (0..2): 2
- Include tracers?: 0
- ISORROPIA coupling (1) / tabulation (0): 0
- Equilibrium calc freq (phys steps, < 5): 1

# Numerical solution parameters

- Physical time steps per hour: 6
[$step] Chemical steps per 1 phys. step : 2, 4
[$ngs] Number of Gauss-Seidel iterations : 1, 1
[$nsu] - during spinup : 5
[$irs] - number of spinup hours : 1
[$iadv] Advection scheme (0..2) : 2
[$iadvv] Vertical advection scheme (0..1) : 1

# Radiative processes
[$ifastj] 0 for old photorates 1 for fastj : 1

# CHIMERE Subgrid Processes
[$ideepconv] Deep convection activation (1/0) : 1
[$urbancorr] Urban correction [1] or not [0] : 0

# Flags whether to run individual dynamic interfaces and the Core
[$imakecompil] Compile dynamic interfaces & core ? : 1
[$imakemeteo] Run meteo interface? (0-2) : 1
[$imakeemis] Build anthropogenic emissions? (0-2) : 1
[$imakedust] Build dust emissions? (0-1) : 1
[$imakerun] Run Chemistry-Transport? (0-1) : 1

# Directories and files (Absolute PATHs here! No stuff like ../../OUTPUTS !)

# Simulation Output
[$simuldir] Simulation output : ${chimere_root}/../BIGFILES/OUTPUTS/${lab}
[$csimuldir] Course run output (for nested run BC) : ${simuldir}/../${clab}
[$psimuldir] Previous run output (if continue) : $simuldir
[$tmplab] Label for date/time of script run : $(date +%Y%m%d_%H-%M)
[$chimere_tmp] Temporary directory : ${simuldir}/tmp${di}-${lab}_${tmplab}

# Static Data
[$bigfilesdir] Big files (AEROMIN.bin, etc) : ${chimere_root}/../BIGFILES
[$iland_cover] Land Cover DB, GLCF(1)/Globcover(2) : 1
[$megan_data] MEGAN data root : ${bigfilesdir}/MEGAN
[$bcdir] Boundary conditions : ${bigfilesdir}/TEST/METEO
[$emissdir] Anthropic emission Dir (from Stage 1) : ${bigfilesdir}/TEST/EMIS
[$fire_emissdir] FIRE emission Dir (from Stage 1) : ${bigfilesdir}/TEST/EMIS

# Dynamic Pre-processors’ Data

# INPUT
[$meteo_DIR] Meteo driver output dir : ${bigfilesdir}/TEST/METEO
[$meteo_file] Meteo file : # ${meteo_DIR}/wrfout_${metdom}_${(date -u +%Y-%m-%d)_00:00:00}
[$meteo_nfile] -“” next file (if WRF continuous run) : # ${meteo_DIR}/wrfout_${metdom}_${(date -u +%Y-%m-%d)_00:00:00}
[$emissdir] Anthropic emission Dir (from Stage 1) : ${bigfilesdir}/TEST/EMIS

# OUTPUT (and possibly input for future runs)
[$datadir] Pre-processors input/output directory : ${simuldir}/data_${dom}_${lab}
[$metdir] Dir to store exdomout file : ${simuldir}/../METEO.${dom}
[$fnmeteo] Meteo out file on chimere 3D grid : ${simuldir}/meteo.${sim}.nc
[$exdomout] METEO file name : ${metdir}/exdomout.${sim1}.nc
${aemisdir} Dir to store anthrpc emiss (stage 2) : ${simuldir}/../AEMIS
${fnemisa} Anthropic emiss. File (from Stage 2) : ${aemisdir}/AEMISSIONS.${sim1}.nc
${fnemisf} Fires emiss. File (from Stage 2) : ${datadir}/FEMISSIONS.${sim}.nc
${fnemisb} Biogenic emission File : ${datadir}/BEMISSIONS.${sim}.nc
${fnemisd} Dust emission File : ${datadir}/DEMISSIONS.${sim}.nc
${iniboundir} Dir to store INI/BOUND fileS : ${simuldir}/../INIBOUN.${dom}.${nbins}
${fnbounconc} Bondary concentrations file : ${iniboundir}/BOUN_CONCS.${sim1}.nc
${fniniconc} Initial concentrations file : ${iniboundir}/INI_CONCS.${sim1}.nc

# ------------ Miscellaneous -----------------------------
${garbagedir} Log files (compilation) : ${chimere_root}/compilogs
${clean} Clean mode : full # full, light, or none

# CHIMERES PARAMETERS SHORT DESCRIPTION
# SEE CHIMERE DOCUMENTATION FOR MORE DETAIL
# ----------------------------
# SOFTWARE REQUIRED: gawk, gmake, netcdf, lam-mpi or openmpi
# A Fortran 90 compiler: CHIMERE has been tested with:
# ifort, pgf90, g95, xlf95
# *** TESTED on architectures: i386/GNU-Linux, x86_64/GNU-Linux, IA64/GNU-Linux
# and power4/AIX-5L
#------------------------------------------
# Chemical parameters of the simulation#
#------------------------------------------
# mecachim:
# [0] : no gas phase chemistry
# [1] : melchior complete
# [2] : melchior reduced
# [3] : SAPRC-07A
# accur=low or full can be used for nesting
# low resolution (main components with families)
# full resolution (all components with families. used for nesting)
# nbins: How many bins for aerosols
# The cut off diameters 2.5 and 10 um are respected.
# You can change the parameter dmax in ./chemprep/chemprep.univ.sh in order to adapt the size distribution. This script is adapted for nbins=4, 6, 12 (nbins=6 is recommended)
# Aerosols: aero flag
2.4 Direct run outputs

2.4.1 The output on screen

The outputs on screen give the correct reading of input file or not, shows the meteorological pre-processing phase and the Chimere simulation itself by printing some variables to give informations about the run. The
choices of outputs are:

- The current date in format yyyymmddhh
- The first two species defined in the OUTPUT_SPECIES file
- The 2m temperature (in Kelvin)
- The boundary layer height (in meters)
- The vertical wind speed (in m/s) of the first vertical level (typically between 0 to 30 m AGL).
- The integration time-step (in mn)
- The percentage of simulation done (in %)
- The CPU used for each hour of simulation (in mn)

All these values are given for a cell located at the middle of the horizontal domain. The results is something like:

<table>
<thead>
<tr>
<th>DATE</th>
<th>O3</th>
<th>NO2</th>
<th>T_2m(K)</th>
<th>PBLH(m)</th>
<th>w(m/s)</th>
<th>DT(mn)</th>
<th>run(%)</th>
<th>CPU(mn)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2013062600</td>
<td>52.3</td>
<td>0.0</td>
<td>30.5</td>
<td>472.</td>
<td>0.69E-03</td>
<td>5.</td>
<td>0.</td>
<td>13.4</td>
</tr>
<tr>
<td>2013062601</td>
<td>52.3</td>
<td>0.0</td>
<td>30.0</td>
<td>470.</td>
<td>0.74E-03</td>
<td>10.</td>
<td>1.</td>
<td>75.8</td>
</tr>
</tbody>
</table>

### 2.4.2 The output files

Four different output files are delivered:

- out**.nc: contains concentrations fields
- meteo**.nc: contains meteorology regridded on the CHIMERE mesh
- dep**.nc: contains dry and wet deposition fluxes
- ini**.nc and end**.nc: for initialization and restart

They are encoded in the NetCDF format, which presents the following advantages:

- portability among different architectures of computers
- self-documentation since a lot of meta-data are included in the file itself
- direct access
- compatibility with many free or commercial post-processing tools

Moreover, CHIMERE uses a NetCDF convention derived from the one used in NCAR’S WRF mesoscale modelling system, simplifying the toolset for post-processing.

### The chemical fields outputs on file "out.[label].nc"

Three-dimensional chemical fields are written in an output out.[label].nc file. The selected species correspond to those listed in the OUTPUT_SPECIES parameter file. Default concentrations values are expressed in ppb. These values may be transformed into $\mu g.m^{-3}$ if the molar mass of each species is added as a second column in the parameter files OUTPUT_SPECIES located in the chemprep directory (the default value is zero).

In case of use of FastJX for the photolysis rates, an output of the optical depth for clouds and aerosols is automatically added as output in the out.[label].nc file.

**example:** In the file chemprep/data/output_species/OUTPUT_SPECIES... located in the chemprep directory (the default value is zero). In case of use of FastJX for the photolysis rates, an output of the optical depth for clouds and aerosols is automatically added as output in the out.[label].nc file.

Selected meteorological and turbulence related fields "meteo.[label].nc"

Hourly 2-D and 3-D meteorological and turbulence related fields calculated on the CHIMERE grid are provided in the output meteo file. For an "off-line" run meteorological fields are calculated with the corresponding meteorological model (e.g. WRF) and then interpolated on the CHIMERE grid. Turbulence related fields are
calculated with the "diagmet" program now embedded in the CHIMERE core. The variables included in the meteo file are listed in Table 2.2.

<table>
<thead>
<tr>
<th>Model Variable</th>
<th>Variable Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Times</td>
<td>Date string</td>
<td>NA</td>
</tr>
<tr>
<td>lon</td>
<td>Longitude</td>
<td>degrees-east</td>
</tr>
<tr>
<td>lat</td>
<td>Latitude</td>
<td>degrees-north</td>
</tr>
</tbody>
</table>

### 2-D Variables

<table>
<thead>
<tr>
<th>Model Variable</th>
<th>Variable Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>hght</td>
<td>Boundary Layer Height</td>
<td>m</td>
</tr>
<tr>
<td>usta</td>
<td>Friction Velocity u_0</td>
<td>m/s</td>
</tr>
<tr>
<td>uwta</td>
<td>Convection Velocity w_0</td>
<td>m/s</td>
</tr>
<tr>
<td>aerr</td>
<td>Aerodynamic Resistance</td>
<td>s/m</td>
</tr>
<tr>
<td>sshf</td>
<td>Surface Heat Flux</td>
<td>W/m²</td>
</tr>
<tr>
<td>slhf</td>
<td>Surface Latent Heat Flux</td>
<td>W/m²</td>
</tr>
<tr>
<td>v10m</td>
<td>10m Zonal Wind Speed</td>
<td>m/s</td>
</tr>
<tr>
<td>w10m</td>
<td>10m Meridional Wind Speed</td>
<td>m/s</td>
</tr>
<tr>
<td>tem2</td>
<td>2m Temperature</td>
<td>K</td>
</tr>
<tr>
<td>soim</td>
<td>Soil Moisture</td>
<td>m³/m³</td>
</tr>
<tr>
<td>sreh</td>
<td>Surface relative humidity</td>
<td>%</td>
</tr>
<tr>
<td>psuf</td>
<td>Surface Pressure</td>
<td>Pa</td>
</tr>
<tr>
<td>swrd</td>
<td>Short Wave Radiation</td>
<td>W/m²</td>
</tr>
<tr>
<td>atte</td>
<td>Radiation Attenuation Coefficient</td>
<td>[0-1]</td>
</tr>
<tr>
<td>copc</td>
<td>Convective precipitation</td>
<td>kg/m²/h</td>
</tr>
<tr>
<td>lspc</td>
<td>Large Scale precipitation</td>
<td>kg/m²/h</td>
</tr>
<tr>
<td>toppc</td>
<td>Total precipitation</td>
<td>kg/m²/h</td>
</tr>
</tbody>
</table>

### 3-D Variables

<table>
<thead>
<tr>
<th>Model Variable</th>
<th>Variable Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>hlay</td>
<td>Top of Layers’ Height</td>
<td>m</td>
</tr>
<tr>
<td>thlay</td>
<td>Layers’ Thickness</td>
<td>m</td>
</tr>
<tr>
<td>winz</td>
<td>Zonal Wind Speed</td>
<td>m/s</td>
</tr>
<tr>
<td>winm</td>
<td>Meridional Wind Speed</td>
<td>m/s</td>
</tr>
<tr>
<td>winw</td>
<td>Vertical Wind Speed</td>
<td>m/s</td>
</tr>
<tr>
<td>temp</td>
<td>Temperature</td>
<td>K</td>
</tr>
<tr>
<td>pres</td>
<td>Pressure</td>
<td>Pa</td>
</tr>
<tr>
<td>airm</td>
<td>Air Density</td>
<td>kg/m³</td>
</tr>
<tr>
<td>sphu</td>
<td>Specific Humidity</td>
<td>kg/kg</td>
</tr>
<tr>
<td>clwc</td>
<td>Liquid (+ice) Water Content</td>
<td>kg/kg</td>
</tr>
<tr>
<td>cliq</td>
<td>Cloud Liquid Water Mixing Ratio</td>
<td>kg/kg</td>
</tr>
<tr>
<td>cice</td>
<td>Ice Liquid Water Mixing Ratio</td>
<td>kg/kg</td>
</tr>
<tr>
<td>rain</td>
<td>Rain Water Mixing Ratio</td>
<td>kg/kg</td>
</tr>
<tr>
<td>kzzz</td>
<td>Vertical Diffusion Coefficient</td>
<td>m²/s²</td>
</tr>
</tbody>
</table>

### Deep convection related fields

<table>
<thead>
<tr>
<th>Model Variable</th>
<th>Variable Description</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>dpeu</td>
<td>Entrainement in Updraft</td>
<td>kg/m²/s</td>
</tr>
<tr>
<td>dped</td>
<td>Entrainement in Downdraft</td>
<td>kg/m²/s</td>
</tr>
<tr>
<td>dpdu</td>
<td>Detrainement in Updraft</td>
<td>kg/m²/s</td>
</tr>
<tr>
<td>dpdd</td>
<td>Detrainement in Downdraft</td>
<td>kg/m²/s</td>
</tr>
<tr>
<td>fluxu</td>
<td>Upward Mass Flux</td>
<td>kg/m²/s</td>
</tr>
<tr>
<td>flxd</td>
<td>Downward Mass Flux</td>
<td>kg/m²/s</td>
</tr>
</tbody>
</table>

### Table 2.2: Variables in the METEO output file.

The deposition fields outputs on file "dep.[label].nc"

This file contains fluxes integrated over the chemical time-step duration. The calculations are done in the model core and are written in independent files. For the dry deposition flux, only the first vertical cell is taken into account. On the other hand, for the wet deposition, fluxes are summed up the whole column since, in the model, each vertical level may contribute to a net sink. Units of these two integrated fluxes are g/cm².

The restart fields outputs on file "end.[label].nc"

The structure of this file is described in Appendix G.7, p.175. The main goal of this file is to save all concentrations fields every 24h. For example, for a second run following in time the first one, this "end..." file will be link to a "ini..." file and thus used to give realistic initial conditions during the restart.

### 2.5 Post-processing the results

Apart some configuration files and static data files written in ASCII code, all the input and output files of the model are written in the NetCDF format, using conventions similar to the WRF conventions. Thus the tools described below may be used to process almost any CHIMERE NetCDF file, including meteo files. CHIMERE NetCDF files are suffixed with .nc.

You can use the CHIMPLET program to visualize your data, either interactively or producing plots automatically. Interactive visualization is done using a simple graphical user interface running chimplot.py. To automate your work you can save a Template after plotting a figure and then run a command-line version chimplotcm.py with a datafile of interest and the generated Template. There are multiple options running chimplotcm.py. Please refer to the CHIMPLET web site for installation and usage guidelines:
2.6 Some figures to validate your first CHIMERE simulation for the 2009 Test Case

Here we present some figures from the March 2009 test case described in §2. If you used the data available on the CHIMERE website for this test case (the TEST directory when using the chimere-download.sh script), and the simulation parameters set by default in chimere.par, then you should obtain the same figures. The figures shown here were made with CHIMPLOT.

To quickly plot these figures with CHIMPLOT you can execute the following few lines of bash code from the main CHIMPLOT directory chimplot. The code runs the command-line utility chimplotcm.py. Sample CHIMPLOT Templates PM10_test.par and wind_test.par are provided with the Test Case and can be downloaded on the CHIMERE download page http://www.lmd.polytechnique.fr/chimere/download.php.

```
chimfile=OUTPUTS/Test/out.20090312_20090319_Test.nc
metfile=OUTPUTS/Test/meteo.20090312_20090319_Test.nc
chimplotcm.py -fig PM10.png "$chimfile $metfile" "PM10_test.par wind_test.par"
```

To make other plots automatically from the template PM10_test.par:

```
for v in NO2 pHNO3 pNH3 pH2SO4 pPPM ; do
    chimplotcm.py -varname "[$v]" -fig $v.png $(chimfile) PM10_test.par
done
```

The code above supposes you put the CHIMPLOT template into the BIGFILES directory containing the OUTPUT directory where the out.*nc file is written.

Note: the "-varname" option can only be used with a single template at a time, therefore the second of the above examples (the one with a loop over species) will plot concentration maps without wind vectors. If you wanted to automate the first of the above examples, please check the templates/mk_templ.py script for template generation.
(a) PM$_{10}$ (µg m$^{-3}$) and NO$_2$ (ppb) concentrations on March 19, 2009 at 12h

(b) HNO$_3$ and NH$_3$ concentrations (µg m$^{-3}$) on March 19, 2009 at 12h

(c) H$_2$SO$_4$ and PPM concentrations (µg m$^{-3}$) on March 19, 2009 at 12h

Figure 2.1: Figures to validate the March 2009 Test Case simulation
Chapter 3

CHIMERE model source code

3.1 CHIMERE general code structure

The general structure of the CHIMERE model is shown in Figure 3.1. Before running the model core (chimere.e executable), a few pre-processors need to prepare the model input data. These are:

- Data generated once per simulation domain $\{\text{dom}\}$ and put to the domains/$\{\text{dom}\}$ directory:
  - Domain horizontal and vertical coordinates (domains/HCOORD/COORD_${\text{dom}}$ and domains/VCOORD/VCOORD_${\text{nlayer_chimere}}{\text{,first_layer_pressure}}{\text{,top_chimere_pressure}}$, see p. 47)
  - Land-use categories: (LANDUSE_[database]_${\text{dom}}$ in ascii format used in chimere and LANDUSE_[database]_${\text{dom}}$.nc to visualize, see p. 48)
  - Biogenic emission factors and leaf-area indices to generate the biogenic emissions with the MEGAN model parameterizations (EFMAP_LAI_${\text{dom}}$.nc, see p. 62)

- Data generated once per specified chemistry/aerosol configuration
  - Chemistry and aerosol parameters (the chemprep/inputdataXXXX.X directory, see p. 53)

- Data from the dynamic pre-processors, often generated for every CHIMERE simulation, but any of them can be re-used for further simulations by adjusting appropriate flags in the top calling script chimere.sh. The following data are put to the CHIMERE data directory $\{\text{datadir}\}$:
  - Emissions: biogenic (BEMISSIONS.${\text{sim}}$.nc, p. 62), anthropogenic (AEMISSIONS.${\text{sim}}$.nc, p. 59), fire emissions (FEMISSIONS.${\text{sim}}$.nc, p. 62) and dust (DEMISSIONS.${\text{sim}}$.nc, p. 63)
  - Meteorological variables (exdomout.${\text{sim}}$.$\{\text{nc}\}$, p. 83)
  - Boundary and initial conditions: BOUN_CONCS.${\text{sim}}$.$\{\text{nc}\}$-* for boundary (p. 77) and INI_CONCS.${\text{sim}}$.$\{\text{nc}\}$-* or end.${\text{sim}}$.$\{\text{nc}\}$ in output directory for initial conditions, depending on whether or not the simulation starts from a restart file (p. 82)

CHIMERE simulation output consists of four NetCDF files in $\{\text{simuldir}\}$:

- Output concentrations out.$\{\text{sim}\}$.$\{\text{nc}\}$
- Restart concentrations end.$\{\text{sim}\}$.$\{\text{nc}\}$
- Depositions dep.$\{\text{sim}\}$.$\{\text{nc}\}$
- Meteorological fields diagnosed by CHIMERE meteo.$\{\text{sim}\}$.$\{\text{nc}\}$ (p. 83)

Each pre-processor prepares its data on the CHIMERE grid and for the time period and region to simulate. The meteorological pre-processor is separated from the rest of the CHIMERE code and is found in the meteo/ directory. It prepares meteorological data in the CHIMERE format on horintal grid (see p. 83). The domain preprocessor is also separated and is found in the domains/ directory (see p. 47). The chemical preprocessor is located in the chemprep/ directory (see p. 53). The rest of the CHIMERE code is in the src/ directory. The model core organization is described below. The main FORTRAN program src/main/chimere.F90 initializes and reads all data and then integrates the model for the required time period. The output files are then
Figure 3.1: General structure of CHIMERE model

available for post-processing. The whole system is driven by the top calling script chimere.sh, which:

- reads parameters of the simulation
- links all necessary files into a temporary directory where all programs are executed
- compiles all necessary code
- runs the 3 dynamic pre-processors (meteo, emission and boundary conditions)
- runs the model itself

Before running the top calling script, it must be edited to specify model options and directories.
Model directories are specified in two different files: data directories are given in chimere.par, while system directories, such as PATHs to NetCDF and MPI libraries, are given in the file mychimere.sh. The latter is activated with a source command inside the top calling script chimere.sh and the compile script. This is done to simplify the model portability between different computers: the user can create one mychimere.[System/Compiler].sh version for each computer, each with its own system PATHs and architecture parameters, and then just create a symbolic link mychimere.sh -> mychimere.[System/Compiler].sh every time one needs to run CHIMERE on one of those computers. This allows to avoid editing system parameters every time the model is run on a different computer or with a different compiler or MPI library.

The script config.sh automates the task of editing mychimere.sh by searching the installed libraries and Fortran compilers and guiding the User to choose between available versions. When making the choices rougeit is up
to User to ensure that all the components are compiled with the same Fortran compiler! After the script has finished its work a new version of mychimere.sh is created corresponding to the desired configuration.

### 3.2 CHIMERE time integration

CHIMERE model is split into two main parts: a general initialization phase and the time integrations of all chemistry-transport equations over the whole simulation duration (Figure 3.2).

![Diagram of CHIMERE time integration](image)

- **The initialization phase** is dedicated to the read of all input parameters as well as the two first meteorological and emissions fields (in order to start the run with realistic meteorological and concentrations fields).
- **The time integration phase** is itself split into three parts:
  - A predefined **hourly time-step**. This time step is fixed and is due to the fact that meteorological and emissions data have to be, at least, hourly provided.
  - A **user’s defined coarse time step 'nphour'**, corresponding to the time interpolation of "physical" parameters, such as wind, temperature, reactions rates etc. A second time-step is dynamically estimated in the meteorological pre-processor. Using the horizontal wind field, the vertical velocity and the entrainment in the updraft (in case of deep convection), a recommended time step is estimated. During the run, if the user time step is too low, the model time integration is increase to reach the recommended value. Figure 3.3 presents preconised 'number of model integration per hor' for the CFL estimated only with the horizontal wind (u), the vertical wind (w) and the entrainment in the updraft (up). For a test run over the CONT5 domain and 10 vertical levels (from surface to 500hPa), with a user time step of 10mn (i.e nphour=6), we can see than deep convection requires to increase the time resolution up to 6mn (i.e nphour=10). If the user’s defined time-step is lower that the recommended one, the user’s choice is applied (even if this is not the optimal choice).
A user’s defined "fine" time step 'ichemstep': this corresponds to the integration of the chemical mechanism, including delta concentrations due to all processes. This is achieved by the two-step scheme. Due to the stiffness of the chemical system to solve, this time step must be at least 30s (or less if possible).

3.3 Directories

The Chimere 2014b top directory contains individual files, the test case top calling script and subdirectories. These subdirectories are:

- **chemprep**: Contains data files for gas, aerosols and chemical mechanisms.
- **domains/**: A subdirectory where coordinate files COORD_${dom} and land-use files LANDUSE_${dom} must be placed for each CHIMERE model domain. This directory contains also the file domainlist.nml where each line corresponds to a model domain.
- **makefiles.hdr/**: Contains examples of Makefile headers suited for several architectures and compilers.
- **meteo/**: This directory contains all the elements for the first step of meteo interfaces, i.e. the horizontal/time interpolation and reformatting of data. When the user starts from a new meteorological data set, a new shell script named interf-${meteo} along with a read/interpolate fortran routine named prep${meteo}.F90 and the associated Makefile-${meteo} should be created by the user and placed in this directory. It is recommended to start from interf-wrf, prepwrf.F90 and Makefile-wrf as templates to help creating these interface programs.
- **scripts/**: Contains families of scripts pointed to by the top level script. While the top level script mainly defines variables, execution scripts in this directory perform the low-level tasks.
- **src/**: Contains the source code of CHIMERE.
- **util/**: Contains some utility programs.

There are other directories created when running the model:

- **exe-${dom}.${nzdoms}.${nmdoms}-${nlayers}**: This is where all executable files are copied. This directory used to not recompile the CHIMERE code at each run.
3.4 Model Files

3.4.1 Scripts

There are three main steps when the top-calling script `chimere.sh` is launched.

1. Preparation of landuse and chemical data files:
   - `chimere-domain.sh` prepares the domain data generated by the static pre-processors
   - `util/define_geom` is an utility script that defines the vertical grid. It outputs a file with hybrid sigma-p coefficients defining the grid.
   - `scripts/define_params.sh` calls `read-params.sh` and `check-dates.sh` to initialize simulation parameters. It is called by `chimere.sh`
   - `chemprep/prep-chemistry-data.sh`, `prep-tracer-data.sh`, `check_consistency.sh`, and `copy-chemresults.sh` rebuild a chemical mechanism (see explanations p.53)
   - `scripts/make-chemistry.sh` is called by `chimere.sh` and prepares chemistry files (if not already done)

2. The sequential part `scripts/chimere-step1.sh`:
   - `scripts/chimere-init.sh` inherits the variables defined in `chimere.sh` and initializes other simulation parameters used by other scripts.
   - `scripts/chimere-compil.sh` is called to compile the model code.
   - `scripts/chimere-bound.sh` launches the initial / boundary conditions interfaces.
   - `scripts/chimere-meteo.sh` launches the meteorological interfaces.
   - `scripts/chimere-aemis.sh`, `chimere-bemis.sh`, and `chimere-dust.sh` perform some sanity checks and launch anthropogenic, biogenic, and dust emission interfaces, respectively.
   - `scripts/chimere-run1.sh` launches the model core execution for the sequential part

3. The parallel part `scripts/chimere-step1.sh`:
   - `scripts/chimere-step2.sh` calls the parallel part of CHIMERE that requires several processors. The separation onto sequential and parallel parts is done to avoid the loss of computing time by requesting many processors on a cluster to run sequential programs.

3.4.2 Makefiles

The compilation process of most of the code in the distribution is driven by Makefiles. To ensure consistency, all Makefile call a unique top level header, `Makefile.hdr`, which deals with all the user installation details.
**Makefile.hdr** is in fact a symbolic link to one of the predefined headers located in **makefiles.hdr** subdirectory.

### 3.4.3 Meteo interface - 1st stage

The interface described below is for WRF, MM5 and ECMWF (noted ecm in `${meteo}` in chimere.par) mesoscale modeling systems. Note that the WRF interface does not require **COORD_${medom}** files, since domain grid coordinates can be found in WRF output NetCDF files and ECMWF interface requires LSMORO file as described below.

1. **meteo/**
   - `compile-meteo.sh`: script to compile the meteorological interface
   - `interf-$\{meteo\}`: scripts to run the meteorological interface

1-1. **meteo/domains/MM5**
   - **COORD_MM5${metdom}**: contains the “cross” coordinates of the MM5 file.
   - **COORD_MM5${metdom}_DOT**: contains the “dot” coordinates of the MM5 file.

1-2. **meteo/domains/ecm**
   - **LSMORO_ecm${metdom}.GRB**: contains the coordinates of the ecm file, Geopotentiel and Land/sea mask at ground.

1-3. **meteo/src/**
   - **${meteo}\_consts.F90**: define uniquely the physical constants used by `prepi${meteo}.F90`.
   - `prepi${meteo}.F90`: read MM5, WRF or emcwf standard output files and perform interpolations to the horizontal CHIMERE model grid. Compiled to `prepi${meteo}.e` and called by the scripts `interf-$\{meteo\}`.
   - **${meteo}\_par.F90**: describes input and output variables for interf-$\{meteo\}$. Should be edited depending on the available variables in the meteo output file.
   - **prep_bilin.F90**: bilinear interpolation subroutine used in the meteo interface `prepi${meteo}.F90`.
   - **Makefile-$\{meteo\}**: Makefiles for the meteo interface compilation.
   - **subs.F90**: contains various helper subroutines (symbolic link to ${chimere_root}/src/tools/subs.F90).
   - **interp_tools.F90**: subroutines to calculate the weighting coefficients for horizontal interpolation (symbolic link to ${chimere_root}/modules/interp_tools.F90).
   - **io.F90**: I/O subroutines (symbolic link to ${chimere_root}/src/tools/io.F90).
   - **calendar.F90**: calendar subroutines (symbolic link to ${chimere_root}/src/tools/calendar.F90).
   - **ncvar.F90**: netcdf I/O subroutines (symbolic link to ${chimere_root}/src/modules/ncvar.F90).

II. **tmpdir/**
   - **${chimere_tmp}/meteo/metargs-$\{meteo\}**: ASCII files generated by the top calling script (`scripts/chimere-meteo.sh`). Passed to `meteo/interf-$\{meteo\}`. Contain parameters to drive `prepi${meteo}.e`.
   - **${chimere_tmp}/meteo/prep${meteo}.nml**: namelist generated by `meteo/interf-$\{meteo\}` to drive `prepi${meteo}.e`.
   - **${datadir}/meteo/exdomout.${sim}.nc**: output NetCDF file generated by `meteo/interf-$\{meteo\}`. Contains meteo variables interpolated to CHIMERE horizontal grid.

III. **util/**
   - **make_mm5_coord**: utility script allowing to extract coordinates and terrain altitude, in longitude/latitude format, of a MM5 **TERRAIN** file. Edit the script itself for giving information. The output files are **COORD_MM5${domain}** and **COORD_MM5${domain}_DOT** used by `interf-MM5`. 
### 3.4.4 Source directories

All the model sources are available in the `src` directory. Some sub-directories are present as follows:

1. **src/** contains source subdirectories and template files
   - `chimere_params.F90.sed` module is a template used to build `chimere_params.F90`. It will hold compile-time parameters of the “master” namespace. Each parameter is defined by a macro, which is substituted before compile time by the top level script.
   - `worker_params.F90.sed` module is a template used to build `worker_params.F90`. It will hold compile-time parameters of the ‘worker’ namespace. Each parameter is defined by a macro, which is substituted before compile time by the top level script.

2. **src/main** contains top level programs
   - `chimere.F90` is the main program. Compiled to `chimere.e` and called by the execution script.
   - `integrun.F90` is the main subroutine called by `chimere.F90` for the “master” process.
   - `master_locvalues.F90` is a subroutine used to calculate time interpolated values in the “master” side.

3. **src/modules** contains master-side modules
   - `chimere_common.F90` module holds all the variables shared in the “master” namespace, type definitions and allocation subroutines.
   - `chimere_consts.F90` module holds most of the physical and mathematical constants used throughout the model.
   - `master_message_subs.F90` module contains a bunch of message passing subroutines, used by the “master” side.
   - `message_defs.F90` module holds constant indexes for message passing between master and workers.

4. **src/initio** contains the initialization and I/O subroutines
   - `ini*.F90` are initialization subroutines executed once by the “master” process.
   - `readhour.F90, renewhour.F90` provide the model with hourly meteo and boundary conditions, under “master” control.
   - `outprint.F90, write*.F90` periodically save the model results to files, under “master” control.
   - `other..*.F90` are helpers for initialization subroutines.

5. **src/model** contains the code for the “workers”
   - `worker.F90` is the main subroutine called by `chimere.F90` for the “worker” processes.
   - `worker_common.F90` module holds all the variables shared in the “worker” namespace, type definitions and allocation subroutines.
   - `worker_message_subs` module contains a bunch of message passing subroutines, used by the “worker” side.
   - `other..*.F90` are the core of CHIMERE model.

Despite the capability of Fortran 95 to perform dynamic memory allocation, CHIMERE still uses static allocation, and ‘common’ declarations, because it proved to be significantly faster at run time.

6. **src/iso** contains the ISORROPIA thermodynamic model. Unmodified ISORROPIA library. Called by workers, but has its own namespace.

7. **src/fastjx70b** contains the Fast-JX model. Called by workers, but has its own namespace.

8. **src/tools** contains helpers. Some helpers, used both by master and workers.

9. **src/prep** contains the code to prepare emissions and boundary conditions before core model run
   - `prepemis.F90` is the standard emission interface. Compiled to `prepemis.e` and called by the top calling script.
   - `prep_bc.F90` is the boundary and initial conditions interface for the coarse (non-nested) runs. Compiled to `prep_bc.e` and called by the top calling script.
• prep_chimere.F90 is the boundary and initial conditions interface for the nested runs. Compiled to prep_chimere.e and called by the top calling script.
• prep_mie.F90 used to initialize (read inputfile) the Fast-JX model. Compiled to prep_mie.e and called by the top calling script.

3.4.5 Dynamic files generated at runtime

All these files are created and moved into the \texttt{tmpdir/} directory.

1. Dynamic parameters
   All these files are created and moved into the \texttt{tmpdir/} directory.
   • \texttt{$(chimere_tmp)/prep_bc.nml}: namelist generated by the top calling script to drive prep_bound.e.
   • \texttt{$(chimere_tmp)/prep_chimere.nml}: namelist generated by the top calling script to drive prep_chimere.e.
   • \texttt{$(chimere_tmp)/prepemis.nml}: namelist generated by the top calling script to drive prepemis.e.
   • \texttt{$(chimere_tmp)/prep_mie.nml}: namelist generated by the top calling script to drive prep_mie.e.
   • \texttt{$(chimere_tmp)/chimere.nml}: namelist containing most of the runtime parameters for the model. This file was the file named INFOS in previous model versions.

2. Dynamic data files
   All these files are created into the \texttt{datadir/} directory.
   • \texttt{$(datadir)/exdomout.$(sim).nc}: NetCDF file generated by the first stage of the meteo interface. Contains meteo parameters interpolated to the model grid.
   • \texttt{$(datadir)/AEMISSIONS.$(sim).nc}: NetCDF file generated by the anthropogenic emissions interface. Contains timely anthropogenic emissions.
   • \texttt{$(datadir)/BEMISSIONS.$(sim).nc}: NetCDF file generated in CHIMERE to save biogenic emissions calculated during the simulation.
   • \texttt{$(datadir)/FEMISSIONS.$(sim).nc}: NetCDF file generated in CHIMERE to save biogenic emissions calculated during the simulation.
   • \texttt{$(datadir)/BOUN_CONCS.$(sim).nc-*}: NetCDF file(s) generated by the boundary/initial conditions interface. Contain timely lateral and top concentrations.
   • \texttt{$(datadir)/INI_CONCS.$(sim).nc-*}: NetCDF file(s) generated by the boundary/initial conditions interface. Contain initial concentrations.

3.5 Routine calls sequence

The general schematic diagram of calls of the CHIMERE model \texttt{chimere.F90} is given in Figure 3.4. Only major routines are cited, not the utility ones.

1. The main program \texttt{chimere.F90} first calls all initialization routines (in inichimere.F90 and further calls) where all "static data" data are read and many variables defined.
2. Then it calls the integration routines \texttt{integrun.F90} and \texttt{worker.F90} which then
   (a) reads hourly data every hour (routine \texttt{readhour.F90})
   (b) loops on the coarse time step,
   (c) outputs results on files (routine \texttt{outprint.F90}) and
   (d) shifts hourly data (routine \texttt{renewhour}).
3. At each model step, one needs hourly data for the start and the end of the hour in order to linearly interpolate, for meteo data, boundary conditions and biogenic emissions. The code keeps only these two instants in memory as explained in Figure 3.5. Within the coarse time step, a call to routine \texttt{physics.F90} is made, in order to define all variables that will be taken as constants during the time step (linear interpolation of meteo data, calculation of reaction rates etc...), and a loop on the fine time step is carried out, with a call to the numerical solver \texttt{twostep.F90}.
Figure 3.4: Detailed list of CHIMERE routines and time loops

4. The `twostep.F90` routine calls the core routine `prodloss.F90` which calculates, for all processes, the loss and production fluxes and sums them. Thus `prodloss.F90` calls `emissions.F90` (emission fluxes), `transmix.F90` (transport and mixing fluxes), `chemistry.F90` (chemical fluxes) and `deposition.F90` (deposition fluxes). The routine `transmix.F90` calculates the PPM concentrations at the boundaries with routines contained in the `ppm.F90` package.

3.6 Parallelism

3.6.1 Domains division

Only the core of the model (chimere.e) has been parallelized. The meteo and preparation interfaces remain sequential tasks.

To allow for a parallel execution of CHIMERE by several processors, the main domain is horizontally divided in rectangular subdomains. This cartesian division is performed in the main execution script, which takes as inputs the user-defined parameters `nzdoms` and `nmdoms`, numbers of subdomains in each dimension. Then the main execution script launches `nzdoms*nmdoms+1` chimere.e processes in parallel, through the MPI command

```
mpirun -np nzdoms*nmdoms+1 ./chimere.e
```

One of these processes will be called the **master**, the others will be **workers**. There are as many workers as CHIMERE subdomains.
Remark: Only \texttt{nzdoms*nmdoms} processors are required to execute the code, because the master process is very light, and is generally working when workers are sleeping. Unless you are not limited in CPU number, don’t waste a CPU for the master and declare only \texttt{nzdoms*nmdoms} in your hostlist file.

In a first order analysis, we could consider that:

1. the master performs all initializations
2. the master sends to each worker its share of data, corresponding to its subdomain
3. the workers work ...
4. the workers send their results to the master
5. the master gathers results, and saves that to output files
6. the master sends new boundary conditions to workers

This would be a beautiful simple world, with birds and flowers ...

In a second order analysis, we realize that a worker process requires not only the share of data corresponding to its subdomains, but also a stripe of boundary data belonging to its neighbours. The reason is that to calculate a target value at point $i$, you need source values at point $i-3$, $i-2$, $i-1$, $i$, $i+1$, $i+2$, $i+3$. In two dimensions, of course.

So, the algorithm becomes:

1. the master performs all initializations
2. the master sends to each worker its share of data, corresponding to its subdomain, plus a surrounding “halo”
3. the workers work, and at each fine time step, update their halo by getting it from their neighbour
4. the workers send their results to the master
5. the master gathers results, and saves that to output files
6. the master sends new boundary conditions to workers

Not so complicated, isn’t it? Let us see where the Devil is hidden ...

In fact, to calculate a target value at point $i$ and time $t_{n+1}$, you need source values at point $i-3$, $i-2$, $i-1$, at time $t_{n+1}$, and source values $i$, $i+1$, $i+2$, $i+3$ at time $t_n$. You cannot simply calculate target values at time $t_{n+1}$ from a set of source values at time $t_n$. That is, to start the calculation of the 5th line of a subdomain,
you need to know the new values of the 3 last pixels of the 5th line of its left neighbour. This is realized by setting a dependancy relationship between lines, and by copying the 3 last pixels of a line to the halo of the corresponding line in the right-hand subdomain. This copy occurs for each line of each subdomain, thus at a frequency much higher than the fine time step.

Last, and hopefully least:
What we have just explained in the previous paragraph for the i direction also applies to the j direction. The dependancy relationship in both directions leads to a straightforward conclusion: it is impossible to parallelize CHIMERE.

We have practically solved the problem by starting the computation of each row of subdomains as if it were an independant domain, with no upper and lower neighbour, exactly as we do for the main domain in the sequential scheme. But at the end of each fine time step, we update their upper and lower halos. This provides a reasonable smoothing between subdomains, albeit not being numerically identical to the sequential scheme. This leads to an imperceptible numerical difference between the results of the sequential model and those of the parallel model, showing patterns parallel to the X direction when we display the difference. The amplitude of the discrepancy is negligible, it damps very quickly, and we have never observed the development of numerical instabilities from these patterns.

### 3.6.2 Recommendations

The optimal number of subdomains \( nzdoms \times nmdoms \) results from a tradeoff between the true computing time and the time wasted in message passing between processes. The message passing time is roughly proportional to the perimeters of the subdomains, and the true computation time to their area. For a 80*80 domain and the gas version, you will waste CPU time in message passing if you go beyond 4*4 subdomains. On the other hand, the same 80*80 simulation with the aerosols version, sea salts and 3 Gauss-Seidel iterations should still be efficient with 8*8 subdomains.

It is the user’s responsibility to try with an increasing number of subdomains (and an increasing number of processors, of course) on a typical forecast configuration, and to decide of the best choice.

Another technical point of detail, which may have severe impacts on performance, is the type of process locking used for collective communications. Suppose that you have divided your domain in 4 subdomains, and you run on 4 processors (defined in your MPI hostlist file). The main calling script will spawn 5 processes: one master, and 4 workers. One processor, generally the first in your hostfile, will be overbooked with the master and the first worker. This is generally not a problem, because master and worker do not work at the same time. But suppose the following case: the master has called the 4 workers, and they have a rendez-vous (synchronization) somewhere in the code. The workers work, and the master sleeps until the program reaches the rendez-vous. No problem, if the master process is really sleeping: the load of the first processor will be 1, produced either by the master, or by the first worker. But if your MPI library has chosen what they call **spin-lock** process locking, the master process will not sleep waiting. It will poll continuously to check if the workers have reached the rendez-vous. In that case, the load of the first processor will be 2: master (polling) and worker1(working) and the whole computing time will be roughly multiplied by 2. With LAM/MPI, this situation is avoided by selecting the **sysv** System Services Interface. This is the rationale of the command

```bash
mpirun -np \$((\$nzdoms*\$nmdoms+1)) -ssi rpi sysv ./chimere.e
```

If you have the opportunity to use many processors for CHIMERE, you can "waste" a processor for the master process. That is, for the 4 subdomains case, you will list 5 processors in your MPI hostlist file. In that case, and only in that case, you can let MPI choose spin-locking for collective communications: it will be faster to have the master polling continuously than awaking it from a real sleep. This is achieved, with LAM/MPI, with this command replacing the previous one:

```bash
mpirun -np \$((\$nzdoms*\$nmdoms+1)) -ssi rpi usysv ./chimere.e
```
3.7 The ’chimere.nml’ model namelist

A CHIMERE run consists in several actions which are performed in the top calling script:

- running the interfaces,
- building the namelists and
- executing ./chimere.e.

For the model execution, many input files are necessary. After running the interfaces, they are listed in the chimere.nml model namelist. This list also contains the output files names and directories. This section describes all files and users choices listed in this namelist. All these input files must be present in the temporary directory before running the executable chimere.e. The top calling script copies and constructs these files in the temporary directory automatically. We also list the corresponding internal file names used during the run. In the following list, we define:

- $modeldir: the model directory
- $tmpdir: the simulation directory
- $outputdir: the output results directory
- $inputdata: an example of chemistry data directory automatically produced by the chemprep script. Note this directory is always produced before a run and always put in the directory $modeldir/chemprep/inputdata
- DOM: an example of simulation horizontal domain
- d1_d2: the starting and ending dates of the simulation
- lab: the name of the simulation

The necessary parameters and input files are listed below. For each file, we describe its "common name", the complete path and its function.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>version</td>
<td>‘chimere’</td>
<td>The model version</td>
</tr>
<tr>
<td>idatestart</td>
<td>2008062100</td>
<td>The starting date of the simulation</td>
</tr>
<tr>
<td>nhourrun</td>
<td>240</td>
<td>The number of hours of the simulation</td>
</tr>
<tr>
<td>ipinit</td>
<td>1</td>
<td>The use of initial conditions</td>
</tr>
<tr>
<td>imakerun</td>
<td>1</td>
<td>Make the run or not</td>
</tr>
<tr>
<td>iusebemis</td>
<td>1</td>
<td>Build biogenic emissions or not</td>
</tr>
<tr>
<td>iusedust</td>
<td>1</td>
<td>Build dust emissions or not</td>
</tr>
<tr>
<td>iusebound</td>
<td>1</td>
<td>Build and use boundary conditions or not</td>
</tr>
<tr>
<td>ifastj</td>
<td>0</td>
<td>Use on-line fastJ scheme or not</td>
</tr>
<tr>
<td>iopt_eros</td>
<td>0</td>
<td>Use local erosion in Europe</td>
</tr>
<tr>
<td>allo_afr</td>
<td>1</td>
<td>Allow emissions of dust in Europe</td>
</tr>
<tr>
<td>icuth</td>
<td>1</td>
<td>The ustar threshold parameterization</td>
</tr>
<tr>
<td>ifluxv</td>
<td>2</td>
<td>The sandblasting flux parameterization</td>
</tr>
<tr>
<td>nlong</td>
<td>95</td>
<td>Number of values in longitude for the dust data</td>
</tr>
<tr>
<td>nlat</td>
<td>24</td>
<td>Number of values in latitude for the dust data</td>
</tr>
</tbody>
</table>

These parameters are integer and describes the starting date and duration (in hours) of the simulation. The other flags are the choices to make the initial conditions, biogenic emissions, mineral dust emissions, the use of boundary conditions, the use of the on-line FastJ module, and the parameterizations included in the mineral dust module.
### Files in the '$inputdata/' directory

The files in the '$inputdata/' directory are produced by the chemprep program during the first model iteration. This includes the active species names, the output species, the stoichiometric coefficients, tables of reaction rates, definition of families, the tabulated zenithal angles, the number of bins, molar weights of aerosols. The specific AEROMIN.bin and AEROORG.bin are binary files for the ISORROPIA and SOA chemical schemes respectively.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>fnoutspec</td>
<td>'inputdata/OUTPUT_SPECIES.full'</td>
<td>Name of output species (here, if the user wants all species in output)</td>
</tr>
<tr>
<td>fnspec</td>
<td>'inputdata ACTIVE_SPECIES'</td>
<td>all active species names</td>
</tr>
<tr>
<td>fnchem</td>
<td>'inputdata/CHEMISTRY'</td>
<td>preprocessed reactions</td>
</tr>
<tr>
<td>fnstoi</td>
<td>'inputdata/STOICHIOMETRY'</td>
<td>stoichiometric coefficients</td>
</tr>
<tr>
<td>fnrates</td>
<td>'inputdata/REACTION_RATES'</td>
<td>tables of reaction rates</td>
</tr>
<tr>
<td>fnfamilies</td>
<td>'inputdata/FAMILIES'</td>
<td>Definition of families</td>
</tr>
<tr>
<td>fnphot</td>
<td>'inputdata/PHOTO_PARAMETERS'</td>
<td>Tabulated zenithal angles</td>
</tr>
<tr>
<td>fnaerosol</td>
<td>'inputdata/AEROSOL'</td>
<td>aerosols; number of bins, molar weights</td>
</tr>
<tr>
<td>fnaeromin</td>
<td>'inputdata/AEROMIN.bin'</td>
<td>Parameters for ISORROPIA scheme for aerosols</td>
</tr>
<tr>
<td>fnaeroorg</td>
<td>'inputdata/AEROORG.bin'</td>
<td>Parameters for the SOA scheme</td>
</tr>
<tr>
<td>fnprim</td>
<td>'inputdata/PRIMARY'</td>
<td>Size distribution of aerosols</td>
</tr>
<tr>
<td>fnsemivod</td>
<td>'inputdata/SEMIVOL.'</td>
<td>Semivolatile aerosols parameters</td>
</tr>
<tr>
<td>fnanthro</td>
<td>'inputdata/ANTHROPIC'</td>
<td>List of anthropic emitted species</td>
</tr>
<tr>
<td>fnfires</td>
<td>'inputdata/FIRES'</td>
<td>List of fires emitted species</td>
</tr>
<tr>
<td>fnbiogen</td>
<td>'inputdata/BIOGENIC'</td>
<td>List of biogenic emitted species</td>
</tr>
<tr>
<td>fndepoespe</td>
<td>'inputdata/DEPO_SPEC'</td>
<td>coefficients for calculation of resistances / species</td>
</tr>
<tr>
<td>fndepopars</td>
<td>'inputdata/DEPO_PARS'</td>
<td>landuse coefficients for dry deposition</td>
</tr>
<tr>
<td>fnwetd</td>
<td>'inputdata/WETD_SPEC'</td>
<td>wet deposition species and parameters</td>
</tr>
</tbody>
</table>

### Files in the domains directory

The files in the domains directory depends only of the horizontal grid. They are automatically generated when the user launch a simulation.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>fnlanduse</td>
<td>'modeldir/domains/DOM/LANDUSE_GLCF_DOM'</td>
<td>Landuse in the CHIMERE classes</td>
</tr>
<tr>
<td>fniVCO</td>
<td>'modeldir/domains/VCOORD/VCOORD_8_997_500'</td>
<td>Vertical coordinates coefficients</td>
</tr>
<tr>
<td>fniMGNEF</td>
<td>'modeldir/domains/DOM/EFMAP_LAI_DOM.nc'</td>
<td>Leaf Area Index for MEGAN</td>
</tr>
<tr>
<td>fnisolpe</td>
<td>'modeldir/chemprep/dustdata/dustdata-soil.asc'</td>
<td>Soil data for dust emissions</td>
</tr>
<tr>
<td>fnisurface</td>
<td>'modeldir/chemprep/dustdata/dustdata-surf.asc'</td>
<td>Surface data for dust emissions</td>
</tr>
</tbody>
</table>

### Output files

The complete format of the main output files is more precisely described in §2.4.2, p.26.
3.8 How to add a variable in the code?

3.8.1 From the master to workers

Using previous versions of the model, to add a new parameter was an easy task. With the parallelized version, this is a little bit more complicated. If you need to know a value in the core model, but using some data estimated with the pre-processors, you need to transfer informations from the master to the workers. Basically, 5 subroutines have to be updated if you want a new variable (real or integer, scalar or array). We present an example based on the deep convection implementation: to know if we are in a convective cell or not, we use a flag named 'ideep(nzonal,nmerid)'. This array has to be hourly updated in the 'locvalues.F90' subroutine (for the estimation of variables at the chemical time-step).

1. src/modules/message_defs.F90:

   integer,parameter :: ias_ideep =__LINE__

2. src/modules/master_message_subs.F90:

   From the master to the worker in send_frac_hourly_int_arrays(ip,dom(ip))

   integer,dimension(:,,:),allocatable :: ibuf2
   allocate(ibuf2(nzcount,nmcount))
   ibuf2=ideep(izstart:izend,imstart:imend)
   call mpi_send(ibuf2, nzcount*nmcount, mpi_integer,ip, ias_ideep, mpi_comm_world,ierr)
   deallocate(ibuf2)

3. src/modules/chimere_common.F90:

   integer,dimension(nzonal,nmerid) :: ideep

4. src/model/worker_common.F90:

   integer,dimension(nzonalmax,nmeridmax) :: ideep

5. src/model/worker_message_subs.F90:

   The worker receives the information from the master in recv_frac_hourly_int_arrays

   integer,dimension(:,,:),allocatable :: ibuf2
   allocate(ibuf2(nzonal,nmerid))
   call mpi_recv(ibuf2, nzonal,nmerid, mpi_integer,0, ias_ideep, &
                 mpi_comm_world,mpi_status_ignore,ierr)
   ideep(1:nzonal,1:nmerid) = ibuf2(:,;)
   deallocate(ibuf2)

3.8.2 From workers to the master

If you need to know the values of a variable calculated in the core worker model (i.e., to write values to an output file), you need to transfer information from the worker to the master, as only the master includes the appropriate subroutines for writing output files. Four source files have to be modified if you want to pass a variable from workers to the master (real or integer, scalar or array).

Consider an example of a photolysis rates variable (phrate worker array) that could be computed in a radiation scheme. Array values are updated hourly, based on clear-sky values per photolysis reaction included in the PHOTO_PARAMETERS file, the zenith angle calculated by the model, and the altitude. Therefore, a 4-dimensional array phrate(nphotmax,nzonal,nmerid,nverti) (nphotmax is the maximum number of photolysis reactions considered in CHIMERE, nzonal is the number of zonal cells for each worker core, nmerid is the
number of meridian cells for each worker core, and nverti is the number of vertical layers) is calculated every hour. With this convention, source files that we need to modify are the following,

1. src/modules/chimere_common.F90:
   Define an array in the master COMMON, with the same type and dimensions as the phrate array,
   
   ```fortran
   real(kind=8), dimension(nphotmax,nzonal,nmerid,nverti) :: phrate
   ```

   The name of this array can be either the same as in the worker (as in this example, phrate) or a different one.

2. src/modules/message_defs.F90:
   Define an integer index for receiving the array by the master:
   
   ```fortran
   integer,parameter :: iar_phrate =__LINE__
   ```

3. src/modules/master_message_subs.F90:
   We usually want to receive the new variable by the master every time it is updated. This updating frequency is essential in order to decide in which master subroutine we should receive the new variable. In this example, phrate is updated hourly so, following the master data flow (see src/main/integrun.F90), the most appropriate master subroutine is,
   
   ```fortran
   subroutine recv_locvalues(ip,dom)
   Since we need a 4-dimensional array buffer, we have to include in this subroutine:
   ```fortran
   Then we call mpi_recv as follows:
   ```fortran
   allocate(dbuf4(nphotmax,nzcount,nmcount,nverti))
call mpi_recv(dbuf4, nphotmax*nzcount*nmcount*nverti, &
    mpi_double_precision,ip, iar_phrate, &
    mpi_comm_world,status,ierr)
phrate(1:nphotmax, izstart:izend, imstart:imend,1:nverti) = dbuf4
deallocate(dbuf4)
   ```fortran

4. src/model/worker_message_subs.F90:
   We have to send the original phrate array values from the worker. Again, following the worker data flow (see src/model/worker.F90), the most appropriate subroutine to do that in the worker in our example is:
   ```fortran
   subroutine worker_send_locvalues
   We have to include in this subroutine:
   ```fortran
   Then we call mpi_send as follows:
   ```fortran
   allocate(dbuf4(nphotmax,nzonal,nmerid,nverti))
dbuf4(:,:,,:) = phrate(1:nphotmax,1:nzonal,1:nmerid,1:nverti)
call mpi_send(dbuf4, nphotmax*nzonal*nmerid*nverti, &
    mpi_double_precision,0, iar_phrate, &
    mpi_comm_world,ierr)
deallocate(dbuf4)
   ```fortran

We highly recommend to understand both integrun.F90 and worker.F90 data flows before applying any of those changes.

### 3.8.3 Write variable into outfile

Consider the same example as before. Phrate worker array is received by master. To write this array into outfile, we need to modify three routines.

1. src/initio/iniconc.F90:
   We need to initialise the phrate array because at the first time step of the simulation this array is not calculated by worker.
2. **src/modules/chimere_common.F90:**
   We have to include in this subroutine:
   ```
   integer :: out_phrate_varid
   ```

3. **src/initio/initio.F90:**
   We have to include in this subroutine:
   ```
   integer :: out_nphot_dimid
   ```
   Then we have to define the new dimension \( nphotmax \) into netcdf file:
   ```
   subroutine create_dims_out
   ncstat=nf90_def_dim(out_ncid,'nphotmax', nphotmax, out_nphot_dimid)
   NCERR(__LINE__)
   Then we have to define the new variable into netcdf file:
   ```
   ! phrate
   ncstat=nf90_def_var(out_ncid,'phrate',NF90_FLOAT, &
      (/out_nphot_dimid,out_zonal_dimid,out_merid_dimid,out_layers_dimid,out_time_dimid/), &
      out_phrate_varid)
   NCERR(__LINE__)
   ncstat=nf90_put_att(out_ncid,out_phrate_varid,'units','K')
   NCERR(__LINE__)
   ncstat=nf90_put_att(out_ncid,out_phrate_varid,'long_name','Temperature')
   NCERR(__LINE__)
   ```

4. **src/initio/outprint.F90:**
   We have to include in this subroutine:
   ```
   real(kind=8), allocatable, dimension(:,,:,:,:) :: toprint4d
   ```
   Then we have to write the new variable into netcdf file:
   ```
   allocate(toprint4d(nphotmax,nzonal,nmerid,nivout))
toprint4d(:,:,1,:,:)=phrate(1:nphotmax,1:nzonal,1:nmerid,1:nivout)
ncstat=nf90_put_var(out_ncid,out_phrate_varid,toprint4d, &
   (/1,1,1,1,iprint+1/),(/nphotmax,nzonal,nmerid,nivout,1/))
NCERR(__LINE__)
deallocate(toprint4d)
```
Chapter 4

[domains]: Domains and landuse

To create a new CHIMERE domain, the User can run either chimere-domain.sh or just the main script chimere.sh, which will call chimere-domain.sh.

Every time you need a new domain, the following steps generally need to be done.

1. Define a new coordinate file domains/HCOORD/COORD_$dom, where $dom is the name of the simulation domain defined in chimere.par.
   - If the new domain is regular in terms of latitude and longitude, just add a line to the domains/domainlist.nml file (see below)
   - Otherwise generate yourself the domains/HCOORD/COORD_$dom file. This file has two columns: "lon lat", and the longitude changes first. You can see the examples in the domains/HCOORD directory.

2. Run chimere-domain.sh. This will
   - Create all landuse data files needed for depositions and biogenic emissions (work done automatically by domains/prep_landuse.sh)
   - Create MEGAN biogenic emission factors and leaf-area indices on the domain grid (work done automatically by domains/prep_megan.sh) for further generation of biogenic emissions by the src/diag/diagbio.F90 program (see p. 62)

3. Create anthropogenic emission files, either on your own, or using the EMEP emissions interface (see p. 59)

The landuse data are automatically calculated. During the first run over a domain, the landuse programs will be launched by the scripts/chimere-domain.sh script and will create all data files for CHIMERE in the domains/$dom directory, where $dom is the name of the simulation domain.

4.1 The domains/domainlist.nml file

If the simulation domain is regular in terms of latitude and longitude, the file domains/HCOORD/COORD_$dom is created automatically from a single line of domain parameters specified by the user in the domains/domainlist.nml file. If the domain already exists, the run continues. Otherwise scripts/chimere-domain.sh calls the domains/makeCOORDdomains.sh script that generates the domain horizontal coordinates in the domains/HCOORD/COORD_$dom file.

For example, the line describing the CHIMERE 'CONT3' domain corresponds to the mesh displayed in the Figure 4.1. The first column, the $dom is a name given by the user to the model horizontal grid/domain. The other columns are the number of cells in the x-direction, the number of cells in the y-direction, and the coordinates of the South-West cell center, as follows:
If, however, the simulation domain is not regular in terms of latitude and longitude, the user has to provide himself a correct `domains/HCOORD/COORD_$dom` file. Note that a domain that is regular in terms of distance (e.g., 3x3 km) is not regular in terms of latitude/longitude.

![Image of horizontal domains](image)

**Figure 4.1**: Examples of horizontal domains. The dots represent the MM5 EUR1 grid cells centers and the rectangle represents the boundaries of the CHIMERE CONT3 domain.

### 4.2 Land Use Types, Data, and Interface

Land use types, or categories, are needed by CHIMERE to calculate a number of processes, such as deposition, biogenic emissions, or surface layer momentum and heat transfer. Land use files need to be constructed only once per model domain. There are currently 9 land use categories in CHIMERE. Those categories are calculated from available global land use databases, which can contain different number of classes. The *chimere 2014b* version comes with land use data and interfaces to two databases: GLCF and GlobCover (see below). The 9 CHIMERE land use types are described in Table 4.1, with the correspondence to the GLCF (University of Maryland) database.

An additional class "inland water" has been added to the classifications in both land cover databases to distinguish between the sea water and fresh water. This was needed to avoid model emissions of sea salt over the fresh water surfaces. The separation was done using a land-sea mask. So instead of the original 14 GLCF and 22 GlobCover classes, CHIMERE land use pre-processor takes 15 and 23 classes for GLCF and GlobCover, respectively (see Table 4.2 and Table 4.3).
Table 4.1: Landuse categories used in CHIMERE

<table>
<thead>
<tr>
<th>Category Number</th>
<th>Description</th>
<th>Corresponding GLCF</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Agricultural land / crops</td>
<td>Cropland</td>
</tr>
<tr>
<td>2</td>
<td>Grassland</td>
<td>Grassland+1/2Wooded grassland</td>
</tr>
<tr>
<td>3</td>
<td>Barren land/bare ground</td>
<td>Bare ground</td>
</tr>
<tr>
<td>4</td>
<td>Inland Water</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>Urban</td>
<td>Urban and built-up</td>
</tr>
<tr>
<td>6</td>
<td>Shrub</td>
<td>Shrublands</td>
</tr>
<tr>
<td>7</td>
<td>Needleaf forest</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>Broadleaf forest</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>Ocean</td>
<td>Water</td>
</tr>
</tbody>
</table>

The Global Land Cover Facility (GLCF)

The Global Land Cover Facility (GLCF) is a 1km × 1km resolution database from the University of Maryland, following the methodology of [Hansen and Reed, 2000]. This global land cover classification is based on the imagery from the AVHRR satellites analyzed to distinguish 14 land cover classes. Table 4.2 shows the 15 GLCF land cover classes used in CHIMERE.

GlobCover Land Cover

The GlobCover Land Cover is a global land cover map at 10 arc second (300 meter) resolution [Bicheron et al., 2011]. It contains 22 global land cover classes defined within the UN Land Cover Classification System (LCCS). GlobCover database is based on the ENVISAT satellite mission’s MERIS sensor (Medium Resolution Image Spectrometer) Level 1B data acquired in Full Resolution (FR) mode with a spatial resolution of 300 meters. GlobCover LC was derived from an automatic and regionally-tuned classification of a time series of MERIS FR composites covering the period December 2004-June 2006. Table 4.3 shows
Table 4.3: GlobCover land cover types used in CHIMERE

The 22 GlobCover classes, together with the additional "Inland water" class, to derive the 9 CHIMERE land use categories.

4.2.1 Land use interface

When the LANDUSE_$dom file is not found in the domains/$dom directory, chimere-domain.sh script runs the land use interface to generate this file.

The scripts and programs are:
- domains/prep_landuse.sh. Runs extract_landuse.e program.
- domains/src/extract_landuse.F90: Extracts original GLCF or GlobCover land cover classes data for the specified Chimere domain from the global data files glcf_world.nc and globcover.nc. Then it calculates the 9-category fractions on the CHIMERE grid from the GLCF or GlobCover classes. It creates LANDUSE_$dom file containing the fraction of land use per grid cell (numbers between 0 and 1, see Table 4.1).

The global land cover NetCDF files glcf_world.nc and globcover.nc are provided in a separate directory. This directory is given by the variable $landcover_dir in the top-calling script chimere.sh. The choice of a land cover Database is made using the script variable $iland_cover: iland_cover=1 for GLCF, land_cover=2 for GlobCover.

ASCII files domains/src/LAND_AGGREGATION_GLCF and domains/src/LAND_AGGREGATION_GLOBCOVER contain the matrix of correspondence between the 15 GLCF classes and the 23 GlobCover classes, respectively, with the 9 CHIMERE categories used by extract_landuse.F90.

The interface contains a new interpolation algorithm that greatly saves computation time when the model
4.3 Details on output files

4.3.1 Horizontal domain COORD

Model domains are entirely defined by their grid cell centres description. It is given in the \texttt{COORD_{\text{dom}}} file which must be placed in the \texttt{domains/} directory. The \texttt{COORD_{\text{dom}}} file contains lines with a longitude (in decimal degree) and a latitude (in decimal degree). Each pair of coordinates stands for a grid cell centre, described (from top to bottom of file) from West to East then from South to North.

In the definition of a new CHIMERE domain, the user must check carefully whether the domain is quasi-rectangular. Most projection systems work, even a regular grid in geographic coordinates (longitude-latitude) provided the resolution is not too coarse (say > 2 degree).

Model grids can be any quasi-rectangular grid, with weakly varying spatial step. It is assumed, in particular for the Parabolic Piecewise Method for transport that locally (over 5 consecutive cells) the grid size is constant in each direction, with sizes equal to that of the locally central cell. Sphericity effects are taken into account, but therefore linearized. It is important to note that the \texttt{COORD} file for CHIMERE is absolutely not the same that the one used for MM5 (or others meteorological inputs). An example is displayed in the Figure 4.1. If the user wants to define his own horizontal grid, we propose a script described in §C.1, p.153.

4.3.2 Vertical grid VCOORD

Structure  The model uses any number of vertical layers, described in hybrid sigma-p coordinates. The pressure in hPa at the top of each layer \( k \) is given by the following formula:

\[
P_k = a_k 10^5 + b_k P_{\text{surf}}.
\]

\( P_{\text{surf}} \) is the surface pressure and the coefficients \( a_k \) and \( b_k \) are calculated by the geom.awk script, called from chimere-domain.sh via define_geom.sh. The \( a_k \) and \( b_k \) coefficients (\( 1 \leq k \leq n_{\text{layer}} \)) are written to the VCOORD file which is then stored in the \texttt{domains/VCOORD/} directory of the chimere root directory, and in the \texttt{domains/} subdirectory of the temporary chimere directory.

The generation of the VCOORD file depends on three parameters of the chimere.par file:

\[
\begin{align*}
\[$n_{\text{layer\_chimere}}$] & \quad \text{Number of vertical layers} : 20 \\
\[$\text{top\_chimere\_pressure}$] & \quad \text{Top layer pressure (mbar)} : 200 \\
\[$\text{first\_layer\_pressure}$] & \quad \text{First layer pressure (sigma * 1e3)} : 997
\end{align*}
\]

\( n_{\text{layer\_chimere}} \) is the number of vertical layers needed, \( \text{top\_chimere\_pressure} \) is the pressure of the top of the domain, and \( \text{first\_layer\_pressure} \) is the pressure of the top of the lowest chimere level, \textit{expressed in } \sigma \times 10^3 \text{ units.}

For example, if \( \text{first\_layer\_pressure} \) is set to 997, the thickness of the first layer (in pressure) will be equal to \( (1 - 0.997) P_{\text{surf}} \simeq 3 \text{ hPa.} \)

Placing the vertical levels  Since version 2014, the algorithm for positioning the vertical levels have changed: up to version 2013b, the layer thickness was increasing exponentially from ground level to the top of the model. Even though this permitted to have a good resolution within the PBL, layers inside the free troposphere had thicknesses reaching several kilometers, which hinders the representation of long-range transportation of anthropogenic of natural contamination plumes (e.g. dust layers). Since version 2014, the algorithm coded in geom.awk produces a VCOORD file in which the thickness of the layers increase exponentially with height in the lowest 200 hPa of the atmosphere, and have constant thickness (in pressure coordinates) from 200 hPa to the top of the model. The number \( n_{200} \) of layers in the lowest 200 hPa of the model is determined so that:
• No layer is thicker than its upper neighbour. Since the layer thickness increase exponentially from $k = 1$ to $k = n_{200}$ and is constant from $k = n_{200} + 1$ to $k = n_{layer\_chimere}$, this condition is equivalent to imposing that layer $n_{200}$ is not thicker than layer $n_{200} + 1$

• $n_{200}$ is the highest possible value such that condition 1 is verified

These two conditions are coded in `geom.awk` and produce a VCOORD file that ensures a fine vertical resolution for the lowest atmospheric layers while not having too thick layers close to model top. Another script `geom-verbose.awk` is also provided in order to make a (relatively) user-friendly output on the screen so that the user can check whether the vertical resolution obtained with their parameters is reasonable. A sample output of `geom-verbose.awk` is as follows:

```
Vertical layers will be as follows :
lowest model layer will be 5 hPa thick
will have 6 layers below 800 hPa
  2 layers from 800 hPa to 500 hPa
k  ca    cb    p(hPa)  thk(hPa)
 1  0.00000 0.99500 995.00000  5.00000
 2  0.00902 0.97705 986.07113  8.92887
 3  0.02513 0.94500 970.12617 15.94496
 4  0.05389 0.88777 941.65206 28.47411
 5  0.10525 0.78555 890.80371 50.84835
 6  0.19697 0.60303 800.00000 90.80371
 7  0.34848 0.30152 650.00000 150.00000
 8  0.50000  0.00000 500.00000 150.00000
```

Users may want to generate their own VCOORD files depending on their modelling priorities (long-range transport, urban boundary layer ...). To do that, the easiest possibility is to modify the `geom.awk` script according to one’s needs.
Chapter 5

[chemprep]: The chemical preprocessor

This is how the chemical preprocessor works.

- When the script chimere.sh is launched, the availability of chemistry input files corresponding to the specific simulation is checked. If the data already exist, the run continues. If not, the script chemprep/make-chemistry.sh creates all prerequisite files.
- This script will create a new directory in the main directory chemprep and called something like inputdata.2110011210.6 where the arguments following the string inputdata correspond to the simulation options. In this new directory, all input files required by CHIMERE for a simulation are stored.
- If a new simulation with the same options is launched or in case of a restart, the files will be used as it. If the main run options change, the script will be automatically launched again to create new files.

5.1 Options available in chimere.par

These options are listed in chimere.par (p.20) under section "Chemistry Options" as follows:

- **mecachim** option for the gas-chemistry mechanism.
  - No gas phase chemistry [0];
  - melchior complete [1];
  - melchior reduced [2];
  - SAPRC-07-A [3]

- **accur** option for the output species accuracy for aerosols\(^1\). Possible values are:
  - low,
  - full.

- **nbins** option for the aerosols bins number.
  - The cut off diameters 2.5 and 10 um are respected.
  - You can change the parameter dmax in ./chemprep/prep-chemistry-data.sh in order to adapt the size distribution.
  - This script is adapted for nbins=4 and nbins=6.

- **aero** options for simulation of aerosols or not.
  - [0=no; 1=yes]
  - (if yes : Minimal configuration with NO3, NH4, SO4, PPM, Sec. Org. Aer., WATER)

- **seasalt** option for the sea salts simulation.
  - none=0,
  - inert=1,
  - active=2.
  - "active" means sea salts react with chemistry

- **iusedust** Mineral dusts are included as active species and emitted within the domain.
[0] if not, [1] if yes.

- **pops**: Persistent Organic Pollutants.
  - pops=1 only if mechim>0 and aero=1

- **carb**: Primary carbonaceous species
  - [0=no; 1=yes]
  - (if yes, OCAR and BCAR are used)

- **trc**: Tracers
  - [0=no; 1=yes]
  - (if yes, both gaseous and particulate tracers can be used)

- **soatyp**: SOA chemistry:
  - no SOA chemistry [0],
  - simple [1],
  - medium [2]
  - Note that soatyp>0 only possible if aero = 1

With these options, the script `scripts/make-chemistry.sh` is launched.

### 5.2 The first-level script `make-chemistry.sh`

This script checks if input data files are already existing or not. If not, new ones are created. The "label" for the output directory is built in this script as follows:

```
labchem=$mecachim $aero $seasalt $pops $carb $gtrc $soatyp $iusedust $iadv $iadvv .$nbins
```

For example and for a simulation with only gas-phase chemistry and no aerosols, but with a passive tracer, the directory created will be with the label "1000001000.0".

### 5.3 The second-level scripts

The script `chemprep/prep-chemistry-data.sh` calls the programs in the directory `chemprep/src`:

- **chemprep-distrib.f**: Program for the calculation of aerosol size distribution. Note that the minimum and maximum value of the aerosols diameters are fixed with the values: $D_{pmin}=0.001\mu m$ and $D_{pmax}=40\mu m$.
  - The user may easily change these values in the `prep-chemistry-data.sh` script.

- **chemprep-families.f**: Reads all species and builds the file containing the name and contents of families.

The script `prep-tracer-data.sh` adds parameters of gaseous and particulate tracers to the data files describing parameters of the chemistry mechanism, depositions, and output: REACTIONS, ANTHROPIC, FAMILIES, DEPO_SPEC, WETD_SPEC, ACTIVE_SPECIES, OUTPUT_SPECIES.full, OUTPUT_SPECIES.low, REACTION_RATES, CHEMISTRY (see below).

### 5.4 Manual changes of the mechanism

The chemical preprocessing scripts allows to modify reactions, add reactions or even completely change the chemical mechanism. It allows an easy writing of reactions and from two initial input files REACTIONS and PHOTORATES produces other files which are read by Chimere. Once the two input files are prepared by the user, the preprocessor is invoked by running the `make-chemistry.sh` script.

The conditions for the set of reactions to be used are listed below:
- Only reactions of the type \( A1(\pm B1(\pm C1,\ldots)) \rightarrow (a^\star)A2+(b^\star)B2+\ldots \) are accepted. Letters with index 1 denote the reactants and those with index 2 the products. \( a, b, (\text{if any}) \) are stoichiometric coefficients. If omitted they are considered to equal 1. Negative stoichiometric coefficients are accepted, but not recommended since it can lead to negative concentrations. Stoichiometry in the reactants is not allowed.
- Only species which are consumed at least once in the mechanism will be considered as active species in the Chimere model. If the user intends to use a species which results of chemical reactions but is not a reactant in any reaction, she (he) should add an artificial reaction to the mechanism, for instance \( A \rightarrow X \) (A is the concerned product), with a negligible reaction rate, i.e. \( k=1e-10 \) (s\(^-1\)).
- There are special species whose concentration is only prescribed in the model. These are H2O (water vapor), N2 (molecular nitrogen), O2 (molecular oxygen) and M (80% N2 + 20% O2). Their values are given by the meteo data. Reaction with these species is possible with no constraint. Changes in these "prescribed species" imply several modifications in the Chimere code and are not an easy issue.
- Reactions have a maximum of 4 reactant species and as many products as desired (less than 1000!). To increase the number of reactants one needs just to change the parameter \( \text{nreactamax} \) in the header files \( \text{src/chimere_params.f90.sed} \) and \( \text{src/worker_params.f90.sed} \).
- It may be desirable that stoichiometric coefficients vary with some parameters like temperature. This is however not possible here in this version.
- All reactions will be processed by the solver in an equivalent manner. There is no family grouping (like often used for the QSSA solver) available.
- Clear sky photolysis rates must be precalculated by the user, and depend only on the zenith angle \( Z \). No dependence on height is allowed, even in the presence of clouds. The proposed tabulated values correspond to an average value between 0 and 1000m. This should be a good compromise for the boundary layer. Introducing a dependence with height will be considered in a future model version. The 12 Tabulated \( J \) values must correspond to zenith angles of (in degree) 90, 88, 86, 83, 80, 75, 70, 60, 45, 30, 15, 0.
- There is a possibility of defining families. These are groups of species whose concentration sum can be output in the model. However these families are only used in outputs, not in the chemistry itself. See syntax in the next section.
- The mathematical expressions for reaction rates (the \( K \)’s and \( J \)’s) can take 20 forms, but here only a limited number is available. The table below shows the available possibilities, together with associated syntax.

<table>
<thead>
<tr>
<th>Type number</th>
<th>Name</th>
<th>Math</th>
<th>syntax in REACTIONS file</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Constant</td>
<td>( K )</td>
<td>( k=\text{value} )</td>
</tr>
<tr>
<td>2</td>
<td>Simplified Arrenius</td>
<td>( K=\text{Aexp(-B/T)} )</td>
<td>( k(T)=\text{Aexp(-B/T)}, A=\text{value, B=\text{value}} )</td>
</tr>
<tr>
<td>3</td>
<td>Arrhenius</td>
<td>( K=\text{Aexp(-B/T)(300/T)**N} )</td>
<td>( k(T)=\text{Aexp(-B/T)(300/T)**N, A=\text{value, B=\text{value, N=\text{value}}} )</td>
</tr>
<tr>
<td>4</td>
<td>Troe or Falloff</td>
<td>( K=\text{K_0*(T**2)/(1+M*(K_0/K_\infty))} )</td>
<td>( K(T,M)=\text{troe(A_0,B_0,N_0,A_\infty,B_\infty,N_\infty,t)} )</td>
</tr>
<tr>
<td>5</td>
<td>Photolysis</td>
<td>( J=J(Z) )</td>
<td>( J(Z)=\text{photorate(label)}^2 ).</td>
</tr>
<tr>
<td>6</td>
<td>Special type</td>
<td>( K=K_1*K_2/(1+K_2) )</td>
<td>( k(T)=\text{SPECIAL}_1(A_1, B_1, A_2, B_2)^3 )</td>
</tr>
</tbody>
</table>

\(^2\text{label} \) is a label standing for recognition of chemprop in the PHOTORATES file. All photolysis rates must appear tabulated in this latter file, the tabulated values corresponding to specific zenith angles (see above)

\(^3\text{Special form for radical recombination (not used in this mechanism)} \)
### 5.5 Syntax of the REACTIONS file

Following are the rules for writing the REACTIONS file:

- Each line is considered as a reaction except blank lines or lines starting with a "#" sign (left for comments).
- Species names must contain at most 15 characters.
- A reaction is written as: \( A1(+A2(+A3(+A4))\rightarrow(a1*)B1+(a2*)B2+(a3*)B3... \) Rate expression where \( Ai \) are the reactants (max=4), \( Bi \) the products and \( ai \) are possible stoichiometric (written if different from 4).

---

4 User can define a new type. Changes must be done in `chemprep.awk` (recognition of a new syntax), `Binichem.awk` (define the number of constant `ltabrate`, and in `Brates.f` (new math expression).

5 Aggregation of the ozone photolysis with reactions with atomic oxygen. The photolysis rates must be those of ozone only, hence the budget reaction is \( O3\rightarrow2*OH \).

6 Fall-off specific to \( NO2+OH+M\rightarrowHNO3 \)

7 User can define a new type. Changes must be done in `chemprep.awk` (recognition of a new syntax), `Binichem.awk` (define the number of constant `ltabrate`, and in `Brates.f` (new math expression).
1). 

- *Rate expression* follows the syntax rules defined in the above table.
- Reactants can also be one (or several) of the prescribed species (H2O, N2, O2 or M).
- A1+A1(+A1)...->... are allowed (repetition of the same reactant, like HO2+HO2...)
- Syntax like A1+A2-A3 is NOT allowed
- Negative stoichiometric coefficients are allowed, but not recommended (correctness of results not guaranteed because never tested). In that case, however, use the syntax ±a1*B1 in the products.
- Families are defined using the syntax:

  \[ \text{FAM}=\text{A1}+\text{A2}+\text{A3}... \]

  \[ \text{Ai} \text{ must be active species, and can be repeated as many times as desired. There is no limitation to the number of family elements.} \]

### 5.6 Syntax of the PHOTORATES file

The syntax is very simple: Each line contains information for one photolysis reaction. There can be more photolysis reactions than in the `REACTIONS` file. The unused ones are ignored. There must be an exact correspondence between the labels of the photolysis reactions defined in the `REACTIONS` file. This label is the first column. The other columns contain the 12 tabulated photolysis rate values for the zenith angles from 90 to 0 degrees (see above table).
Chapter 6

Emissions

CHIMERE accounts for four types of emissions:

- **Anthropogenic emissions** that need pre-processing by the user either with an inventory and model of his/her own or, for emissions over Europe with the stand-alone model developed and distributed by the CHIMERE team (Sect. 6.1).
- **Biogenic and natural emissions** that if not provided by the user may be automatically calculated with the embedded CHIMERE pre-processor based on landuse data (Sect. 6.2).
- **Dust emissions** that may also be estimated with the embedded CHIMERE pre-processor (Sect. 6.3)
- **Fire emissions** that need pre-processing by the user following a stand-alone procedure (Sect. 6.4)

6.1 Anthropogenic surface emissions

There are two options on how anthropogenic emissions may be handled by the CHIMERE model. The user can pre-process anthropogenic emissions from an inventory of his/her own choice and input directly the “AEMISSIONS.{sim}.nc” ready-to-read netCDF file to CHIMERE (see Appendix G.4, p.172) (Sect. 6.1.1). Alternatively, CHIMERE team develops and distributes an anthropogenic surface emission pre-processing model called emiSURF that based on a top-down approach estimates hourly emission fluxes on the CHIMERE grid and the period of the simulation from the EMEP data over Europe (Sect. 6.1.2). The output of this model may be processed by the anthropogenic emission pre-processor embedded in CHIMERE (“prepemis.F90”), which compiles the “AEMISSIONS.{sim}.nc” file.

6.1.1 User’s precompiled emissions

The user should compile his/her own AEMISSIONS.nc file. This file must contain hourly emission fluxes, projected on the CHIMERE 3-D grid for all gases and aerosol species involved in the chemical mechanism of the CHIMERE simulation (MELCHIOR or SAPRC) in molecules cm$^{-2}$ s$^{-1}$ (see Table 6.1 for the list of the required species may). Aerosol fluxes should also be converted in “molecule-like” units in this anthropogenic emission input file considering a fictitious molar mass equal to 100 g mol$^{-1}$. The conversion coefficient from mass unit to CHIMERE model unit is $6.022 \times 10^{23}$ mol$^{-1}/(100 \text{ g mol}^{-1})$. In this case the user should set the [$imakeaemis$] flag at 0, so that “prepemis.F90” program does not run, and provide the appropriate [aemisdir] and [fnemisd] paths pointing to the AEMISSIONS.{sim}.nc file in the “chimere.par” file.

6.1.2 The emiSURF interface

For simulations over Europe, the starting point are annual national emission totals from the EMEP database (EMEPCWEST [V. Vestreng, 2005]) available at the web site http://www.emep.int. Additional data for benzo(a)pyrene, benzo(k)fluoranthene and benzo(b)fluoranthene (respectively BaP, BkF and BbF) can
MELCHIOR2

<table>
<thead>
<tr>
<th>NO</th>
<th>Nitrogen monoxide</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO2</td>
<td>Nitrogen dioxide</td>
</tr>
<tr>
<td>HONO</td>
<td>Nitrous acid</td>
</tr>
<tr>
<td>SO2</td>
<td>Sulphur dioxide</td>
</tr>
<tr>
<td>NH3</td>
<td>Ammoniac</td>
</tr>
<tr>
<td>CO</td>
<td>Carbon monoxide</td>
</tr>
<tr>
<td>CH4</td>
<td>Methane</td>
</tr>
<tr>
<td>C2H6</td>
<td>Ethane</td>
</tr>
<tr>
<td>NC4H10</td>
<td>n-Butane</td>
</tr>
<tr>
<td>C2H4</td>
<td>Ethene</td>
</tr>
<tr>
<td>C2H6</td>
<td>Ethane</td>
</tr>
<tr>
<td>C3H6</td>
<td>Propene</td>
</tr>
<tr>
<td>C5H8</td>
<td>Isoprene</td>
</tr>
<tr>
<td>OXYL</td>
<td>o-Xylene</td>
</tr>
<tr>
<td>HCHO</td>
<td>Formaldehyde</td>
</tr>
<tr>
<td>CH3CHO</td>
<td>Acetaldehyde</td>
</tr>
<tr>
<td>CH3COE</td>
<td>Methyl ethyl Ketone</td>
</tr>
<tr>
<td>APINEN</td>
<td>α-pinene</td>
</tr>
</tbody>
</table>

AEROSOLS

<table>
<thead>
<tr>
<th>PPM_fin</th>
<th>Primary particulate matter</th>
</tr>
</thead>
<tbody>
<tr>
<td>PPM_coa</td>
<td>Primary particulate matter</td>
</tr>
<tr>
<td>PPM_big</td>
<td>Primary particulate matter</td>
</tr>
<tr>
<td>H2SO4_fin</td>
<td>Primary sulfuric acid</td>
</tr>
<tr>
<td>BaP_fin</td>
<td>Benzo(a)pyrene</td>
</tr>
<tr>
<td>BbF_fin</td>
<td>Benzo(b)fluoranthene</td>
</tr>
<tr>
<td>BkF_fin</td>
<td>Benzo(k)fluoranthene</td>
</tr>
<tr>
<td>OCAR_fin</td>
<td>Primary organic carbon</td>
</tr>
<tr>
<td>BCAR_fin</td>
<td>Primary black carbon</td>
</tr>
</tbody>
</table>

SAPRC

| CH4 | Methane                  |
| CO  | Carbon monoxide          |
| HONO| Nitrous acid             |
| NO  | Nitrogen monoxide        |
| NO2 | Nitrogen dioxide         |
| SO2 | Sulphur dioxide          |
| ACET| Acetone                  |
| ALK1| Ethene                   |
| ALK2| Propane                  |
| ALK3| Alkans 2.5×10^3<k_OH<5×10^3|
| ALK4| Alkans 5×10^3<k_OH<1×10^4 |
| ALK5| Alkans 1×10^4<k_OH        |
| AR01| Aromatiques k_OH<2×10^4  |
| AR02| Aromatiques k_OH>2×10^4  |
| BALD| Aromatic aldehydes       |
| CCHO| Acetaldehyde             |
| C2H4| Ethene                   |
| GLY | Glyoxal                   |
| HCHO| Formaldehyde              |
| MACR| Methacrolein             |
| OLE1| Alkens k_OH<7×10^4       |
| OLE2| Alkens k_OH>7×10^4       |
| CRES| Phenols and Cresols      |
| PRD2| Ketones (k_OH>0.7×10^5 ppm^−1 mn^−1) |
| RCCHO| Lumped C3+ Aldehydes     |
| CSH8| Isoprene                 |
| APIEN| α-pinene                 |
| ACYE| Acetyl en                 |
| BENZ | Benzen                   |
| AACD| Acetic Acid               |
| IPRD | Lumped isoprene product species |
| NH3 | Ammoniac                  |

Table 6.1: Gas and particle emissions required for MELCHIOR and SAPRC

be requested on the EMEP-MSCEAST web site [http://www.msceast.org](http://www.msceast.org). Annual totals for European countries are provided per SNAP sector in Mg-year^−1·grid cell area^−1 over the 0.5°×0.5° resolution EMEP grid. The following pollutants are available: NO₂, SO₂, NMVOC, CO, NH₃, PM^ coarse =PM₁₀−PM₂.₅, where PM^coarse =PM₁₀−PM₂.₅. Inventory data are provided for each year and can be found in the annual-EMEP05x05/data_expert directory. The processing of the annual totals to obtain hourly fluxes over the CHIMERE 3-D grid for all the chemical species of the corresponding mechanism consists in three main steps in the emiSURF model (Figure 6.1).

Step 1 [emep_preproc.sh]
This bash shell program reads the annual inventory data and creates one file per pollutant: NO₂, SO₂, NMVOC, CO, NH₃, PPM2 = PM^ coarse and PPM3 = PM₂.₅. The header of these files reads: COUNTRY_ID, WE_EMEP_cell_ID, SN_EMEP_cell_ID, SNAP1,...,SNAP10. Emission fluxes are in Mg-year^−1·EMEP grid cell area^−1.

Step 2 [source2chimere.F90]

- Spatial allocation of surface emissions on the CHIMERE grid is based on landuse data. Two databases
Figure 6.1: **Top-down processing of EMEP anthropogenic emissions with the emiSURF interface**

are implemented in the current version of emiSURF: glcf data at 1km resolution developed by the University of Maryland Department of Geography ([http://www.landcover.org](http://www.landcover.org)) and globcover at 10 arc second (≈300m) resolution developed under the European Space Agency initiative ([http://due.esrin.esa.int/globcover/](http://due.esrin.esa.int/globcover/)). In both cases emiSURF spatially allocates emissions based on a classification among four landuse types: urban, crop, water or forest.

- Annual data for each inventory pollutant are allocated on the twelve months of the year based on seasonal factors provided by the Institute of Energy Research for each country and SNAP sector (see the inputdata/SEASONAL-FACS_<POL> file).
- A second temporal allocation is applied to account for day-of-week variation, per pollutant, country and SNAP sector (see the inputdata/WEEKLY-FACS_<POL> files), where columns read from Monday through Sunday. These variations follow the guidelines provided by the Institute for Energy Economics and Rational Use of Energy, University of Stuttgart; [Ebel et al., 1994]

- A time-shift on the data is applied to take into account the time zone and daylight saving information for each country.
- 24-hour profiles for each day of week and for each SNAP sector are applied over the emissions to obtain hourly data.
- Hourly emissions from all SNAP sectors, gridded over the CHIMERE simulation domain are aggregated to a single flux per emitted pollutant.
- Chemical speciation operates on the emitted pollutants at two stages. “Inventory” pollutants (i.e PPM2, PPM3, NOx, CO, SOx, NH3, CH4 and NMVOC) split into “real” compounds with ratios depending on the SNAP activity sector. At a second stage, “real” compounds split into “model” compounds depending on the chemical mechanism (Melchior or SAPRC). This process is described in the AGGREGATION_$mechanism files found in the “inputdata” directory. Differences between the two chemical mechanisms apply only to the NMVOC species.

**NOx:** For all SNAP sectors 90% of NOx emissions is assigned to NO2, 9.2% to NO and 0.8% to HONO [R. Kurtenbach, 2001]. Depending on the country, NOx emissions in the EMEP inventory may include soil NO biogenic emissions in the “Agriculture” sector. The user should be careful not to doublecount NO soil emissions when running the biogenic emissions pre-processor embedded in the CHIMERE model (Sect. 6.2).

**SOx:** For all SNAP sectors, 99% of SOx is assigned to SO2 and 1% to sulphuric acid (H2SO4) in the particulate phase.

**NMVOC:** For both mechanisms (Melchior and SAPRC) NMVOC emissions first split into 221 “real” compounds of the british PORG speciation depending on the SNAP sector [Passant, 2002]. Then, a two-step procedure aggregates “real” VOC compounds to a smaller set of VOC classes which correspond...
directly to the specific compounds of the MELCHIOR or SAPRC chemical mechanism, following the Middleton methodology [Middleton et al., 1990]. Following this procedure, “real” compounds are lumped together into “model” compounds using a reactivity weighting factor which depends on the relative OH radical rate constants of the “real” and “model” compounds. The user should bear in mind that the same reactivity weighting factors are used on emissions for all countries, which represents a significant source of uncertainty in the spatial distribution of VOC emissions.

**AEROSOLS:** The coarse and fine fractions of particles (PPM2 and PPM3 respectively) split into PPM_coa and PPM_fin, BCAR_coa and BCAR_fin and OCAR_coa and OCAR_fin at ratios depending on the SNAP activity sector. **NEW:** The speciation of the carbonaceous species has changed in chimere2014. When the carb parameter is set to 1 in chimere.par, the anthropogenic species are separated into PPM, OCAR, and BCAR in CHIMERE. Otherwise, if carb=0, the non-carbonaceous species PPM are mixed with OCAR and BCAR resulting in the species called TPPM. For all the activity sectors H$_2$SO$_4$ emissions (1% of the total SO$_x$) is attributed to the fine mode H$_2$SO$_4$_fin.

### 6.2 Biogenic emissions

#### 6.2.1 The biogenic emitted species

In the complete version of the model, the model needs:

- **NO** ................. Nitrogen monoxide
- **C5H8** ....................... Isoprene
- **APINEN** .................... α-pinene
- **BPINEN** ................... β-pinene
- **LIMONE** .................. Limonene
- **TERPEN** .................. Terpene (Lumped class)
- **OCIMEN** ............. Ocinene (Lumped class)
- **HUMULE** .......... Humulene (Lumped class)
- **H2SO4_coa** .............. Total dry sea salts
- **SALT_coa** .............. Chloride fraction of sea salts
- **NA_coa** ............ Sodium fraction of sea salts
- **HCL_coa** .......... Chloride fraction of sea salts
- **H2SO4_coa** .............. Sulfate fraction of sea salts
- **WATER_coa** ........ Water fraction of sea salts
- **OCIMEN** ............. Ocinene (Lumped class)
- **HUMULE** .......... Humulene (Lumped class)
- **H2SO4_coa** .............. Sulfate fraction of sea salts
- **WATER_coa** ........ Water fraction of sea salts
- **OCIMEN** ............. Ocinene (Lumped class)
- **HUMULE** .......... Humulene (Lumped class)
- **H2SO4_coa** .............. Sulfate fraction of sea salts
- **WATER_coa** ........ Water fraction of sea salts

Emissions of six Chimere species: isoprene, α-pinene, β-pinene, limonene, ocmene, and NO, are calculated using the MEGAN model data and parameterizations. The new MEGAN model ([Guenther et al., 2006], v. 2.04) exploits most recent measurements in a gridded and canopy scale approach, more appropriate for use in CTMs since it estimates the effective burden of gases that mix and react in the boundary layer. Estimates of biogenic VOCs from vegetation and NO emissions are calculated as:

$$ ER_i = EF_i \times \gamma_i(T, PPFD, LAI) \times \rho_i $$ (6.1)

where $ER_i$ ($\mu g.m^{-2}.h^{-1}$) is the emission rate of species $i$, $EF_i$ ($\mu g.m^{-2}.h^{-1}$) is an emission factor at canopy standard conditions, $\gamma_i$ (unitless) is an emission activity factor that accounts for deviations from canopy standard conditions, and $\rho_i$ is a factor that accounts for production/loss within canopy. The canopy standard conditions relevant for this study are defined as: air temperature (T) of 303 K, photosynthetic photon flux density (PPFD) of 1500 $\mu mol.m^{-2}.s^{-1}$ at the top of the canopy, leaf area index (LAI) of 5 $m^2.m^{-2}$ and a canopy with 80% mature, 10% growing and 10% old foliage. The MEGAN model parameterizes the bulk effect of changing environmental conditions using three time-dependent input variables specified at top of the canopy: temperature (T), radiation (PPFD), and foliage density (LAI). The production/loss term within canopy is assumed to be unity ($\rho = 1$). The equation can then be expanded as:

$$ ER_i = EF_i \times \gamma_{T,i} \times \gamma_{PPFD} \times \gamma_{LAI} $$ (6.2)

The MEGAN model provides input EF and LAI data over a global grid, hereafter projected on the CHIMERE model grid. The current available choice for EFs is restricted to following species: isoprene, α-pinene, β-
pinene, myrcene, sabinene, limonene, $\delta^3$-carene, ocimene, and nitrogen oxide. EF’s are static and refer to years 2000-2001. They are obtained summing up over several plant functional types (e.g. broadleaf and needle trees, shrubs, etc...). LAI database is given as a monthly mean product derived from MODIS observations, referred to base year 2000. Hourly emissions are calculated using 2-m temperature and short-wave radiation from a meteorological model output. The optimal choice for this work is the 150” resolution products proposed in the MEGAN inventory. The daily PPFD and temperature, which are representative values of the simulation, are set to the fixed values of 400. $\mu mol.m^{-2}.s^{-1}$ and 297 K, respectively.

Terpene and humulene emissions are not calculated in this model version and are set to zero. Sea salt emissions are calculated by [Monahan, 1986]:

$$dF = \frac{1.373 r^{3.41} r^{-3} (1 + 0.057 r^{1.05}) 10^{1.19} e^{-B 2}}{0.65}$$

(6.3)

$$B = 0.38 \log(r) - 0.65$$

(6.4)

$F$ is the flux of sea salt particle number in particles $m^{-2} s^{-1} \mu m^{-1}$, $r$ the particle radius in $\mu m$ and $U_{10}$ is the wind speed at 10 m in m s$^{-1}$.

### 6.2.2 Biogenic emission interface

The **BEMISSIONS.nc** required by the model file should contain 2D hourly biogenic emissions with Isoprene, Terpenes and Nitrogen Monoxide. It is created by the src/initio/write_bemis.F90 program. The format of the **BEMISSIONS.nc** netCDF file is given in Appendix G.5, p.174, with 2D records containing the biogenic emission rates in molec/cm$^2$/s.

- The program **remap_ef.F90** called by **prep_megan.sh** interpolates original global MEGAN emission factors and LAI data on the Chimere grid for the required domain. **prep_megan.sh** is called by **make-chemgeom.sh**, so these calculations can be done only once for a given domain. Original emission factor data are netcdf files called <spec>all200021.nc corresponding to the period 2000–2001 with <spec> referring to a given species. Those files must be stored in the $bigfilesdir/MEGAN/NETCDF_150sec/EF/EFMT21b directory. LAI data are 12 netcdf files of the format laivyyyymm.nc each file corresponding to one month of the year. The files must be stored in the $bigfilesdir/MEGAN/NETCDF_150sec/LAI/LAI20 directory. The output file is called **EFMAP_LAI_<domain>.nc** and is put to the **domains** directory. It contains emission factors for each MEGAN species, as well as 12 LAIs for each month as 2D variables on the Chimere grid for the given domain.

- Module **diagbio_megan** in src/model/diagbio_megan.F90 contains subroutine **megan_bioemis** called from src/model/worker_bio.F90 that calculates emission rates for the nine afore-mentioned MEGAN species (redistributed into the six Chimere species) using parameterizations of the original MEGAN code [Guenther et al., 2006]. The module also contains the data used for the calculations.

- Biogenic emissions for sea salts are calculated in the **calculate_bioemissions** subroutine from src/model/diagbio_science.F90 module, which is called by src/model/worker_bio.F90. The file **LANDUSE_<domain>.nc** that contains land use fractions (see **Table 4.1**) is required for sea salt calculations by **calculate_bioemissions**.

### 6.3 Mineral dust emissions

This CHIMERE model version may be viewed as an intermediate one concerning a complete mineral dust emissions calculation over Europe and Africa. Historically, there was no dust emissions in CHIMERE before 2005.

Between 2005 and 2008, two model developments were done in parallel:
• a simple dust emissions scheme for Europe, in order to close the aerosol mass budget for air quality studies ([Vautard et al., 2005b]). This development was done over Europe only due to the availability of anthropogenic emissions (EMEP only for the CHIMERE version previous to 2008). The parameterization were chosen to be simple in order to ensure fast calculations considering that all gaseous and particles species are calculated. The main goal was not to have the best emissions schemes but a scheme able to unbiase the modelled aerosols masses over Europe, and enough robust and stable to make confident forecasts.

• the transport model CHIMERE-dust dedicated to long range transport of dust over the northern hemisphere ([Menut et al., 2005, Menut et al., 2007, Menut, 2008, Menut et al., 2013]). This model was developed for studies of mineral aerosols processes (emissions and transport) over the Northern Atlantic.

In 2010, the development of CHIMERE-dust was frozen. Its specific parameterizations were implemented into CHIMERE (specific dry deposition velocities, saltation and sandblasting, Weibull distribution for wind speed used for emissions, the Tiedke deep convection scheme). The current model version thus proposed the two models into a single one. However, the developments are not yet finished: the mineral dust database used is only valid for arid and semi-arid areas over Africa (Figure 6.2) and the erosion scheme over Europe remains simple. For the next years, developments will be done to ensure an homogeneous mineralogic and soil database over the globe and a single saltation and sandblasting scheme.

Dust emissions are calculated by the src/model/worker_dust.F90 program. The latter uses diag-dust_science.F90 module.

6.3.1 Dust emissions over Africa

We used the scheme presented by [Alfaro and Gomes, 2001] to compute the dust fluxes and the size distribution. The calculations are numerically optimized following the developments in [Menut et al., 2005]. Table 6.2 displays notations, their values (if constants) and related units we used for the calculations. This model described the dust emission process as a balance between the kinetic energy provided by the saltating soil grains and the cohesion energy of the dust particles. The complete dust emission model proposed by [Alfaro and Gomes, 2001] is a coupling of the saltation flux calculation proposed by [Marticorena and Bergametti, 1995], and the sandblasting model developed by [Alfaro et al., 1998].
### Parameter Notation Unit

#### Surface layer dynamic parameters
- Wind speed at 10 meters AGL: $U_{10m}$ m.s\(^{-1}\)
- Saltation roughness length: $z_0$ m
- Smooth erodible roughness length: $z'_0$ m
- Saltation friction velocity: $u_s$ m.s\(^{-1}\)
- Threshold saltation friction velocity: $u^*_T$ m.s\(^{-1}\)

#### Soil characteristics
- Soil particle density [quartz grains]: $\rho_p$ kg.m\(^{-3}\)
- Air density: $\rho_{air}$ kg.m\(^{-3}\)
- Soil aggregate particle size diameter: $D_p$ m
- Particle kinetic energy: $e_c$ kg.m\(^2\).s\(^{-2}\)
- Threshold saltation friction velocity: $u^*_T$ m.s\(^{-1}\)

#### Multimodal aerosol size (with $i$ values\(*\))
- Mean Mass Diameter: $d_{m,i}$ m
- Geometric standard deviation: $\sigma_i$ ad.
- Binding energy: $e_i$ kg.m\(^2\).s\(^{-2}\)

#### Fluxes (with $j$ values\(*\))
- Aerosol bin mass diameter: $d_{m,j}$ m
- Horizontal (saltation) flux: $F_h$ kg.m\(^{-1}\).s\(^{-1}\)
- Mass vertical (sandblasting) flux: $F_{v,m}$ kg.m\(^{-2}\).s\(^{-1}\)
- Number vertical (sandblasting) flux: $F_{v,n}$ m\(^{-2}\).s\(^{-1}\)
- Sandblasting efficiency (for mass): $F_{v}/F_h \alpha$ m\(^{-1}\)
- Adaptative constant: $\beta$ m.s\(^{-2}\)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Notation</th>
<th>Unit</th>
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<tbody>
<tr>
<td>Surface layer dynamic parameters</td>
<td>$U_{10m}$</td>
<td>m.s(^{-1})</td>
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<tr>
<td>Wind speed at 10 meters AGL</td>
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<tr>
<td>Saltation roughness length</td>
<td>$z_0$</td>
<td>m</td>
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<tr>
<td>Smooth erodible roughness length</td>
<td>$z'_0$</td>
<td>m</td>
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<tr>
<td>Saltation friction velocity</td>
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<td>m.s(^{-1})</td>
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<tr>
<td>Threshold saltation friction velocity</td>
<td>$u^*_T$</td>
<td>m.s(^{-1})</td>
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<tr>
<td>Soil characteristics</td>
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<td>Soil particle density [quartz grains]</td>
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<td>Air density</td>
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<td>Soil aggregate particle size diameter</td>
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<td>Particle kinetic energy</td>
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<td>Multimodal aerosol size (with $i$ values(*))</td>
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<td>Mean Mass Diameter</td>
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<td>$e_i$</td>
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<td>Fluxes (with $j$ values(*))</td>
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<td>Aerosol bin mass diameter</td>
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<td>Horizontal (saltation) flux</td>
<td>$F_h$</td>
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<td>m(^{-2}).s(^{-1})</td>
</tr>
<tr>
<td>Sandblasting efficiency (for mass)</td>
<td>$F_{v}/F_h \alpha$</td>
<td>m(^{-1})</td>
</tr>
<tr>
<td>Adaptative constant</td>
<td>$\beta$</td>
<td>m.s(^{-2})</td>
</tr>
</tbody>
</table>

Table 6.2: Notations used to describe the saltation and sandblasting processes. * $i=3$ in this case.

#### 6.3.1.1 Saltation flux

As described in [Marticorena and Bergametti, 1995], [Alfaro and Gomes, 2001], [Gomes et al., 2003], the vertically integrated saltation flux is estimated using the [White, 1986]'s equation:

$$F_h(D_p) = \frac{K \rho_{air}}{g u_s} \left(1 - \frac{u^*_T}{u_s}\right) \left(1 + \frac{u^*_T}{u_s}\right)^2$$  \hspace{1cm} (6.5)

where $u_s$ is the "saltation" friction velocity, i.e the friction velocity calculated using the roughness length, $z_0$, following [Marticorena and Bergametti, 1995]. $u^*_T$ is the threshold friction velocity depending on the soil particle diameter size $D_p$ and $z_0$. Following [Marticorena and Bergametti, 1995], we consider the air density as constant with $\rho_{air}=1.227$ kg.m\(^{-3}\), and used the constant value $K = 1$. The parameterization used for the calculation of $u^*_T$ is the one proposed by [Shao and Lu, 2000]:

$$u^*_T(D_p) = \sqrt{a_n \left(\frac{\rho_p g D_p}{\rho_{air}} + \frac{\gamma}{\rho_{air} D_p}\right)}$$ \hspace{1cm} (6.6)

with the constant parameters $a_n = 0.0123$ and $\gamma=300$ kg.m\(^{-2}\). The particle density, $\rho_p=2.65 \times 10^3$ kg.m\(^{-3}\) is chosen to be representative of quartz grains clay minerals.

The threshold friction velocities $u^*_T$ may be modified by the drag partitioning and the soil moisture. In this study, we used the drag partitioning proposed by [Marticorena and Bergametti, 1995] without soil moisture influence.

The saltation flux $F_h$ is non-zero only if $u_s > u^*_T(D_p)$ for a given soil particle diameter $D_p$. The total saltation flux is thus obtained by integrating $F_h$ over the soil size distribution from $D_p^{min}=10^{-6}$m to $D_p^{max}=2.10^{-2}$m.
This interval is chosen in order to cover the whole range of possible soil sizes.

### 6.3.1.2 Sandblasting flux

The sandblasting fluxes is computed based on the partitioning of the kinetic energy of individual saltating aggregates and the cohesion energy of the dust particles. This model assumed that dust emitted by sandblasting is characterized by three modes whose proportion depends on the wind friction velocity. From wind tunnel measurements performed on two natural soils from semi arid regions, [Alfaro et al., 1998] consider these three modes as independent of the soil types. They described the three modes using log-normal distributions with diameters $d_1=1.5 \times 10^{-6}$ m, $d_2=6.7 \times 10^{-6}$ m and $d_3=14.2 \times 10^{-6}$ m and their associated standard deviation, respectively $\sigma_1=1.7$, $\sigma_2=1.6$ and $\sigma_3=1.5$. Based on this model, as soil aggregate size or wind speed increases, kinetic energy becomes able to release first particles of the coarsest mode that are associated with the lowest cohesion energy, then particles from the intermediate population, and finally the finest particles. It also implied that for a specific wind speed and soil size distribution, the dust flux may be zero even if the saltation process occurs. In order to apportion the available kinetic energy between the three modes, a constant cohesion energy $e_i$ is associated to each mode values. The numerical values of $e_i$ were determined by adjusting the predicted aerosols size distribution to those measured in wind tunnel under different wind conditions, using an iterative least square routine, as described in [Alfaro et al., 1998]. Depending on the description of the soil size distribution (measured or fitted), this procedure leads to different values of the cohesion energy [Alfaro et al., 1998]. [Alfaro and Gomes, 2001] recommend the use of the following values: $e_1=0.376$, $e_2=0.366$ and $e_3=0.346$ kg.m$^2$s$^{-2}$.

<table>
<thead>
<tr>
<th>$e_i$</th>
<th>$p_1$</th>
<th>$p_2$</th>
<th>$p_3$</th>
</tr>
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<tbody>
<tr>
<td>$e_c &lt; e_3$</td>
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<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$e_3 &lt; e_c &lt; e_2$</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
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<tr>
<td>$e_1 &lt; e_c$</td>
<td>$\frac{e_c-e_1}{e_c-e_3}$</td>
<td>$(1-p_1)\frac{e_c-e_2}{e_c-e_3}$</td>
<td>$1-p_2-p_3$</td>
</tr>
</tbody>
</table>

Table 6.3: Fractions ($p_i$) of the kinetic energy for the three binding energies $e_i$, after [Alfaro et al., 1997]

The kinetic energy is expressed, as a function of the soil particle diameter after [Alfaro et al., 1997] and [Shao and Lu, 2000]:

$$e_c = \rho_p \frac{100\pi}{3} D_p^3 (u_*)^2$$  \hfill (6.7)

It is compared to cohesion energy of the three aerosol modes in order to compute the proportion $p_i(D_p)$ of these three modes to the total dust size-distribution (Table 6.3). The variations of $p_i(D_p)$ as a function of the available kinetic energy are illustrated in Figure 6.3. Once the kinetic energy exceed $e_3$, the coarse mode is release and $p_3$ remains equal to 1 when the kinetic energy increase until it reaches $e_2$. Then $p_3$ exhibit a sharp decrease for any further increase of the kinetic energy. On the opposite, $p_2$ increase rapidly from 0 to 0.60 between $e_2$ and $e_1$. The decrease of $p_2$ once $e_1$ has been reached is not so severe than for $p_3$.

The dust flux is assumed to be proportional to the horizontal salination flux $F_{h}(D_p)$. After [Alfaro and Gomes, 2001], summing the Equation 6.8 over the three aerosols modes, the total sandblasting flux may be written:

$$F_{v,m,i}(D_p) = \sum_{k=1}^{N_{class}} \frac{\pi}{6} \rho_p \beta \frac{p_i(D_p,k)d_{m,i}^3}{e_i} \int dF_{h}(D_p,k)$$  \hfill (6.8)
where $N_{\text{class}}$ is the number of intervals discretizing the soil size distribution in the range $[D_{p}^{\text{min}} : D_{p}^{\text{max}}]$ and $d_{m,i}$ the mean mass diameter.

Finally, these three mass fluxes contributions are redistributed into the aerosols bins. The discretization chosen for aerosol size distribution ranged from $10^{-7}$ m to $10^{-4}$ m with 100 bins for this work. The corresponding mass fraction is distributed using a log-normal distribution, [Seinfeld and Pandis, 1998].

### 6.3.1.3 Weibull distribution for 10m wind speed

The interest of the specific Weibull distribution to represent wind speed variability was extensively discussed by numerous authors such as [Pavia and O’Brien, 1986], [Pryor et al., 2005] and [Cakmur et al., 2004]. In order to build a distribution for a chosen wind speed value, representing the mean value for a specific area and period, the probability density function is expressed as:

$$p(|U|) = \frac{k}{A} \left( \frac{|U|}{A} \right)^{k-1} \exp \left[ -\left( \frac{|U|}{A} \right)^{k} \right]$$  \hspace{1cm} (6.9)

where $k$ is a dimensionless shape parameter (in our case $k = 4$) and $A$ is a scale parameter related to the mean of the distribution (in our case the modelled wind speed for each cell and each modelled hour).

### 6.3.1.4 The smooth roughness length and drag partition factor

The smooth roughness length, $z_{0_s}$, is calculated only for coarse sand, fine-medium sand and silt because clay is too fine and does not represent erodible material. It is defined, for each soil type as the maximum among the three diameters (coarse sand, fine-medium sand and silt) and which have a non-zero mineral fraction, divided by 30. The smooth roughness length is required in the drag partition factor computation [Marticorena and Bergametti, 1995].

### 6.3.2 Dust emissions over Europe

The goal for dust over western Europe was not to develop a sophisticated erosion scheme for temperate regions as described in [Vautard et al., 2005b]. The parameterization follows the classical approach of dust emission
modelling in a simplified manner. The dust vertical flux (in g.m$^{-2}$.s$^{-1}$) $F$ is modelled with a functional approach similar to that of [Zender et al., 2003], which itself is based on the [Marticorena and Bergametti, 1995] approach and the [White, 1986] formula:

$$F = \alpha C u_{ss} (u_{ss}^2 - u_{st}^2)$$  \hspace{1cm} (6.10)

where $u_{ss}$ denotes the saltation friction velocity, $u_{st}$ the threshold friction velocity and $C$ is a coefficient that may depend on several surface factors. The sandblasting efficiency, $\alpha$, describes the ratio of the vertical flux to the horizontal saltation flux. The saltation friction velocity $u_{ss}$ corresponds to that encountered on erodible parcels of the model grid cell, usually smoother than typical vegetated surfaces found in Europe. It is calculated by using the 10m wind field, a saltation roughness length of $5.10^{-4}$m and the assumption of neutral stability as in most previous studies. In order to keep the formulation simple, the threshold friction velocity is assumed to depend only on gravimetric soil moisture $w$. This dependence uses the [Fecan et al., 1999] formulation:

$$u_{st} = f_w u_{st0}$$  \hspace{1cm} (6.11)

where $u_{st0}$ is the minimal friction velocity for dust entrainment over dry soil, and is taken to be uniformly constant. The soil moisture factor $f_w$ is given by

$$
\begin{cases}
  w < w_t & f_w = 1 \\
  w > w_t & f_w = \sqrt{1 + 1.21(100(w - w_t))^{0.68}}
\end{cases}
$$  \hspace{1cm} (6.12)

where $w_t$ is the gravimetric soil moisture content (in kg.kg$^{-1}$) above which entrainment is inhibited by soil moisture. This threshold is usually calculated as a function of the fraction of clay, in a rather empirical manner. In Europe during the summer season, the volumetric soil moisture provided by the NCEP GFS analyses and MM5 drops below 0.15 (gravimetric equivalent of about 0.10) only after several weeks without precipitation. We take here the uniform constant value $w_t = 0.1$ kg.kg$^{-1}$ throughout the model domain, which corresponds to a large clay fraction ([Fecan et al., 1999]).

The independence of threshold friction velocity on soil type is a strong assumption, since our aim is only to test the impact of introducing erosion processes. [Iversen and White, 1982] and [Shao and Lu, 2000] have proposed formulations linking the threshold velocity to the soil particle distribution. In both cases a minimal value of 0.2 m.s$^{-1}$ is found, related to soil particles with a mean diameter of 0.1 mm. According to [Xuan, 2004], threshold friction velocities adjusted to wind tunnel observations are too large as they do not account for subgrid scale turbulence. Following this argument we divided the previous minimal threshold by 2 and take $u_{st0} = 0.1$ m.s$^{-1}$.

The sandblasting efficiency is taken as $\alpha = 510^{-5} m^{-1}$ an order of magnitude obtained from the measurements, over Northern Spain and Niger, of [Gomes et al., 2003], and it is again kept uniformly constant, although its dependence can be made explicit as a function of clay content ([Marticorena and Bergametti, 1995]).

In the ideal case of a bare, non crusted soil, the factor $C$ has been taken equal to ([Zender et al., 2003]):

$$C_i = \frac{2.61 \rho_{air}}{g}$$  \hspace{1cm} (6.13)

In practice, the soil is covered with vegetation, snow or water over most of Western Europe and is very often crusted. We, therefore, define:

$$C = f_c f_b C_i$$  \hspace{1cm} (6.14)

where $f_c$ is the crustation factor, which has been found from field studies to lie in the 0.001-0.1 range ([Goossens, 2003]; [Gomes et al., 2003]), and $f_b$ is the fraction of bare ground where dust is available for entrainment. In practice, the product $f_c f_b$ is taken here uniformly constant over land and is tuned to optimize
the model/observation correlations while keeping the average mineral dust fraction close to that found in the climatological observations of [Putaud et al., 2004]. This leads to $f_c f_b = 410^{-3}$: This strong assumption of a uniform factor leads to a large uncertainty. However, our results remain valid if other factors of the same order of magnitude are taken. Due to this uncertainty, our results should be considered in a qualitative manner only, which is enough for a sensitivity study. The [Fecan et al., 1999] parameterization of the effect of soil moisture was unable to inhibit dust erosion in sporadic events of fall wind and rain storms over Western Europe under wet conditions. Dust emissions are therefore set to zero when gravimetric soil moisture exceeds 0.2, and kept as the scheme calculates them only when it is below 0.16, a linear interpolation being performed between these two values.

The above emissions are assumed to be total emissions. Since emissions of mineral dust occurs primarily in the coarse mode, one assumes half of emissions in the 10-40 $\mu$m mode, 45% of emissions in the 2.5 $\mu$m mode and the remaining 5% are distributed in the fine mode using the same distribution as for anthropogenic.

![Figure 6.4: Relative part of the most important soil class for each model cell. A value of 0.5 means that the most present soil represents 50% of the model cell.](image)

### 6.3.3 Data used for the mineral dust emissions calculations

The model parameters presented in Table 6.4 are mandatory to estimate mineral dust emissions fluxes.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Units</th>
<th>Time variability</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soil composition (over Africa only)</td>
<td>% clay, % silt, % sand</td>
<td>constant</td>
</tr>
<tr>
<td>Aeolian roughness length $z_0$ (over Africa only)</td>
<td>cm</td>
<td>constant</td>
</tr>
<tr>
<td>Erodibility (over Africa only)</td>
<td>%</td>
<td>constant</td>
</tr>
<tr>
<td>10m wind speed</td>
<td>m/s</td>
<td>variable</td>
</tr>
</tbody>
</table>

**Table 6.4: Needed parameters for the mineral dust emissions fluxes calculations**

The soil is represented by relative percentages of sand, silt and clay for each model cell. Over Africa, data are built using ERS scatterometer data for $z_0$, USGS and STATSGO-FAO data for landuse and soil properties. The spatial coverage is limited to the Northern Africa as displayed in Figure 6.4. The data are available in the CHIMERE file: chemprep/dustdata/dustdata-surf.asc.

For each soil type, mineralogical properties are defined as:

- coarse sand: $D_p=0.069 \mu$m, $\sigma=1.6$
• fine medium sand: $D_p=0.021 \, \mu m$, $\sigma=1.8$
• silt: $D_p=0.0125 \, \mu m$, $\sigma=1.6$
• clay: $D_p=0$, $\sigma=0$

These parameters are not dependent on time nor meteorology and are considered as constant. Based on these primary soil properties, more refined soil species are defined as explained in Table 6.5. An $\alpha$ factor is also defined, leading to estimate the vertical dust flux using the [Marticorena and Bergametti, 1995] scheme but not the explicit [Alfaro and Gomes, 2001]. However, it is strongly recommended to use [Alfaro and Gomes, 2001] to retrieve realistic vertical fluxes. These data are available in the input CHIMERE data file: chemprep/dustdata-soil.asc.

<table>
<thead>
<tr>
<th>[Marticorena and Bergametti, 1995] soiltypes</th>
<th>Category</th>
<th>% CS</th>
<th>% FMS</th>
<th>% silt</th>
<th>% clay</th>
<th>% salt</th>
<th>$\alpha$</th>
<th>$z_{0s}$</th>
<th>Soiltype</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>62.5</td>
<td>37.5</td>
<td>0</td>
<td>0</td>
<td>6.15e-06</td>
<td>7.00e-04</td>
<td></td>
<td>silty fine sand</td>
</tr>
<tr>
<td>2</td>
<td>80</td>
<td>20</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1.25e-06</td>
<td>2.30e-03</td>
<td></td>
<td>medium sand</td>
</tr>
<tr>
<td>3</td>
<td>100</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1.00e-06</td>
<td>2.30e-03</td>
<td></td>
<td>coarse sand</td>
</tr>
<tr>
<td>4</td>
<td>90</td>
<td>10</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1.12e-06</td>
<td>2.30e-03</td>
<td></td>
<td>coarse medium sand</td>
</tr>
<tr>
<td>5</td>
<td>0</td>
<td>100</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>3.04e-06</td>
<td>7.00e-04</td>
<td></td>
<td>fine sand</td>
</tr>
<tr>
<td>6</td>
<td>31.25</td>
<td>31.25</td>
<td>37.5</td>
<td>0</td>
<td>0</td>
<td>4.35e-06</td>
<td>2.30e-03</td>
<td></td>
<td>silty medium sand</td>
</tr>
<tr>
<td>7</td>
<td>0</td>
<td>0</td>
<td>20</td>
<td>0</td>
<td>80</td>
<td>4.04e-06</td>
<td>1.73e-03</td>
<td></td>
<td>salty medium sand</td>
</tr>
<tr>
<td>8</td>
<td>0</td>
<td>0</td>
<td>8</td>
<td>0</td>
<td>92</td>
<td>3.18e-06</td>
<td>1.73e-03</td>
<td></td>
<td>salty silt fort</td>
</tr>
<tr>
<td>9</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>100</td>
<td>0</td>
<td>0.0e+00</td>
<td>2.30e-03</td>
<td></td>
<td>Clavey soil</td>
</tr>
<tr>
<td>10</td>
<td>0</td>
<td>0</td>
<td>50</td>
<td>0</td>
<td>50</td>
<td>7.35e-06</td>
<td>1.73e-03</td>
<td></td>
<td>Salt waste</td>
</tr>
<tr>
<td>11</td>
<td>0</td>
<td>0</td>
<td>100</td>
<td>0</td>
<td>0</td>
<td>1.99e-05</td>
<td>4.17e-04</td>
<td></td>
<td>Agricultural soil</td>
</tr>
<tr>
<td>12</td>
<td>0</td>
<td>0</td>
<td>50</td>
<td>0</td>
<td>10</td>
<td>3.50e-06</td>
<td>1.73e-03</td>
<td></td>
<td>Salty fine sand</td>
</tr>
<tr>
<td>13</td>
<td>60</td>
<td>0</td>
<td>40</td>
<td>0</td>
<td>0</td>
<td>3.31e-06</td>
<td>2.30e-03</td>
<td></td>
<td>Silty Coarse Sand</td>
</tr>
<tr>
<td>21</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td>Mountains, cities</td>
</tr>
<tr>
<td>22</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td>Rivers</td>
</tr>
<tr>
<td>23</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td>Cultures</td>
</tr>
<tr>
<td>24</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td>Inland water</td>
</tr>
<tr>
<td>99</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.0</td>
<td>0.0</td>
<td></td>
<td>Ocean</td>
</tr>
</tbody>
</table>

Table 6.5: Description of soil types. CS= Coarse sand; FMS=Fine medium sand.
6.4 Fire emissions

To account for fire emissions in the CHIMERE simulations, the following lines need to be informed in `chimere.par`:

- `$fire_emissions` should be set to 1;
- `$fire_emissdir` is the name of the directory where fire emissions are stored;
- `$fnemisf` is the name of the output emission file.

Species list is the same as the anthropogenic one in the current version.

Fire emissions have to be provided in the following file format:

- One netcdf file per species and per month;
- Hourly emissions gridded on the simulation domain;
- Emissions are only provided for grid cells with non-zero values, as a list of sources
- List of variables:
  - `lon`: Longitude grid (2D)
  - `lat`: Latitude grid (2D)
  - `ilatsources`: Latitude index of non-zero sources (1D=sources)
  - `ilonsources`: Longitude index of non-zero sources (1D=sources)
  - `SPEC`: Hourly emissions for species SPEC (3D=hours,days,sources) in molecule/cm²/s

Example netcdf file header for CO is given in Appendix G.8.
Chapter 7

Depositions and resuspension

7.1 Dry deposition

7.1.1 For gases:

Dry deposition is considered for model gas species \(i\) and is parameterized as a downward flux \(F_{d,i} = -v_{d,i}c_i\) out of the lowest model layer with \(c_i\) being the concentration of species \(i\). The deposition velocity is, as commonly, described through a resistance analogy ([Wesely, 1989]):

\[
v_{d,i} = \frac{1}{R_a + R_{b,i} + R_{c,i}}
\]

(7.1)

Stable case

\[
R_a = \frac{1}{ku_*} \left[ \ln \left( \frac{z}{z_0} \right) + 4.7(\zeta - \zeta_0) \right]
\]

(7.2)

Neutral case

\[
R_a = \frac{1}{ku_*} \left[ \ln \left( \frac{z}{z_0} \right) \right]
\]

(7.3)

Unstable case

\[
R_a = \frac{1}{ku_*} \left[ \ln \left( \frac{z}{z_0} \right) + \ln \left( \frac{(\eta_0^2 + 1)(\eta_0 + 1)^2}{(\eta_r^2 + 1)(\eta_r + 1)^2} \right) + 2 \left( tan^{-1} \eta_r - tan^{-1} \eta_0 \right) \right]
\]

(7.4)

where \(\eta_0 = (1 - 15\zeta_0)^{1/4}\), \(\eta_r = (1 - 15\zeta_r)^{1/4}\) and \(\zeta_0 = z_0/L\). \(L\) is the Obukov length, \(k\) the von Karman constant and \(z_0\) is the dynamical roughness length. \(z_0\) depends on the fraction of land-use for each category and on the season. See Section on land-use and on meteorology for more details.

According to [Hicks et al., 1987] the quasi laminar resistance \(R_{b,i}\) is calculated as:

\[
R_{b,i} = \frac{2}{ku_*} \left( \frac{Sc_i}{Pr} \right)^{2/3}
\]

(7.5)

where \(Sc_i\) and \(Pr\) are the Schmidt and Prandtl number, respectively, \(k\) the von Karman’s constant and \(u_*\) the friction velocity.

The formulation of the surface resistance \(R_c\) follows [Erisman et al., 1994]. It uses a number of different other resistances accounting mainly for stomatal and surface processes which are again dependent on the land use type and season. Necessary chemical parameters for the calculation of \(R_c\) are also taken from [Erisman et al., 1994] except for carbonyls ([Sander et al., 1999]; [Baer and Nester, 1992]) and peroxide
species ([Hall et al., 1999]). All species-related parameters are gathered in the DEPO_SPEC file located in all chemprep/inputdata directories related to the simulation.

In the DEPO_SPEC parameter file:

```
O3  48  0.01  1  2000
SO2  64  1e5  0  1e-20
NO2  46  0.01  0.1  2000
NO  30  2e-3  0  2000
NH3  17  1e+5  0  1e-20
```

These columns are read and used in the `initio/inidepo.f90` subroutine. The parameters are:
1. charspec: species name
2. dMx: molar mass of the model species
3. dHx: effective Henry’s law constant (M atm$^{-1}$) for the gas
4. df0: a normalized (0 to 1) reactivity factor for the dissolved gas
5. rRwat: parameter is not used

In `initio/inidepo.f90`, dHx and df0 are used for the mesophyllic resistance value (definition in [Seinfeld and Pandis, 1998], p.973) as:

- **Mesophylle resistance Rm factor**
  ```
  do nd=1,ndepo
     Rm(nd)=1d-2/((dHx(nd)/3d3)+(1d2*df0(nd)))
  enddo
  ```

- **Quasi-laminary boundary layer resistance Rb factor**
  ```
  do nd=1,ndepo
     DH2O_Dx=sqrt(dMx(nd)/18d0)
     factRb(nd) = ((rNu/(DH2O*prandtl)) &
                   * (DH2O_Dx)**(2d0/3d0) &
                   * 2d0/vkarm
  enddo
  ```

Here DH2O and DH2O_Dx are the molecular diffusivity of water and gaseous species, respectively.

The main land/seasonal parameters can be found in the file DEPO_LAND file which can be found in all chemprep/inputdata directories. Seasonal variations of resistances are taken from 3 Wesely Seasons:

- **#1** (summer with full vegetation), from may to october. In August, September and October, however, LAI, stomatal resistance and deposition height are divided by two for the CROPLAND category in order to take into account harvested fields.
- **#3** (winter without frost) from november through march.
- **#5** (transitional season with short annuals) for April.

Most land parameters are taken from [Wesely, 1989], but LAI are drawn from the NASA/EOSDIS Oak Ridge National Laboratory using average LAI field measurements, for Summer.

Dry deposition (for gases) parameters are initialized in routine `src/initio/inidepo.f90`. At the coarse time step frequency, deposition velocities are calculated in routine `src/model/depvel.f90`. Deposition fluxes are calculated at the fine time step frequency in routine `src/model/deposition.f90`.

### 7.1.2 For aerosols:

Dry deposition for aerosols also makes use of a resistance scheme. The dry deposition velocity is expressed as:
\[ v_d = v_s + \frac{1}{r_a + r_b + r_a r_b v_s} \]  

(7.6)

where \( v_s \) is the sedimentation velocity expressed as in [Seinfeld and Pandis, 1998], \( R_a \) the aerodynamic resistance and \( R_b \) the quasi-laminar resistance for particles. The aerodynamic resistance \( R_a \) is calculated as the integral of the inverse of the diffusivity coefficient \( K(z) \) up to the middle of the model surface layer, which can be estimated using the analytical formulae of the surface-layer similarity profiles for \( K \) ([Seinfeld and Pandis, 1998]). Over vegetal canopies, corrections have been implemented according [Zhang et al., 2001], [Giorgi, 1986] and [Peters and Eiden, 1992]. A complete discussion on mechanistic processes of dry deposition is available in [Petroff, 2005].

### 7.2 Wet scavenging

When the aerosol option is selected, scavenging for gas/aerosols in clouds or rain droplets is taken into account. Wet scavenging is formulated as follows:

- **For gases in clouds**: Nitric acid, ammonia in the gas phase are scavenged by cloud droplets. This process is assumed to be reversible. Moreover, for in-cloud scavenging, dissolved gases in a non precipitating cloud can reappear in the gas phase due to cloud dissipation. Equilibrium between dissolved gases concentration and gas-phase concentrations follow Seinfeld and Pandis (1998).

  \[ \Gamma = \frac{p D_g}{6.10^3 u_g D^2} (2 + 0.6 R_e^{1/2} S_{c}^{1/3}) \]  

(7.7)

\( p \) being the precipitation rate (mm h\(^{-1})\), \( D_g \) the molecular diffusion coefficient (m\(^2\)s\(^{-1}\)), \( u_g \) the raindrop velocity (m s\(^{-1}\)), \( R_e \) and \( Sc \) respectively the Reynolds and Schmidt numbers of drops. [Mircea and Stefan, 1998] and references therein give relationships between \( u_g \) and hydrometeor diameter for various types of precipitation. In the model, sulfur dioxide and hydrogen peroxide are also scavenged by precipitation.

- **For particles in clouds**: Particles can be scavenged either by coagulation with cloud droplets or by precipitating drops. Particles also act as cloud condensation nuclei to form new droplets. This latter process of nucleation is the most efficient one in clouds. According to [Tsyro, 2002] and [Guelle et al., 1998], the deposition flux is written as:

  \[ \left[ \frac{dQ^k_i}{dt} \right] = -\frac{\epsilon_i P_r}{w_l h} Q^k_i \]  

(7.8)

with \( P_r \) being the precipitation rate released in the grid cell (g cm\(^{-2}\) s\(^{-1}\)), \( w_l \) the liquid water content (g cm\(^{-3}\)), \( h \) the cell thickness (cm) and \( \epsilon_i \) an empirical uptake coefficient (in the range 0 - 1) depending on particle composition. \( l \) and \( k \) are respectively the bin and composition subscripts.

- **For particles in rain droplets below the clouds**: Particles are scavenged by raining drops, the deposition flux of particles being:

  \[ \left[ \frac{dQ^k_i}{dt} \right] = -\alpha p E_l \frac{Q^k_i}{u_g} \]  

(7.9)

with \( \alpha \) being an empirical coefficient, \( P \) the precipitation rate in the grid cell (g cm\(^{-2}\) s\(^{-1}\)), \( E \) a collision efficiency coefficient between particles and raining drops ([Loosmore and Cederwall, 2004]) and \( u_g \) the falling drop velocity (cm s\(^{-1}\)).
7.3 Resuspension of particulate matter

Text published in [Vautard et al., 2005b]

Saltation, which is necessary to transfer small mineral particles from the soil into the atmosphere, is not the only natural aerosol upward entrainment process. Resuspension of freshly deposited small particles lying at the surface by turbulent wind is a distinct process, their extraction resulting from the imbalance between adhesive and lifting forces (see e.g. [Reeks and Hall, 2001]). Such particles can originate from the atmosphere or the biosphere, and are particularly easy to extract shortly after deposition ([Loosmore, 2003]). They can be made of vegetal debris obtained from the mechanical or biological degradation of canopy elements, spores, pollens, etc. ([Simoneit and Mazurek, 1982]). The evidence of the presence of biogenic non mineral compounds in the continental aerosols has been reported several times (see e.g. [Andreae and Crutzen, 1997], for instance in the form of "humic matter", consisting in carbonaceous polymers (see [Gelencser et al., 2002] and references therein), and cellulose ([Kunit and Puxbaum, 1996]). As shown by [Gelencser et al., 2002], some of these aerosols could be of secondary nature. However, for the sake of simplicity, we assume that this biogenic aerosol component is of primary origin. In order to represent these processes, we use a bulk formulation based on the simple resuspension rate empirical formula of [Loosmore, 2003], which was shown to provide a very good fit to the available resuspension measurement data:

\[
\lambda = 0.01 \frac{u_*^{1.43}}{\tau^{1.03}}
\]  

(7.10)

where \( \lambda \) is the resuspension rate (in s\(^{-1}\)) and \( \tau \) is the time after the start of resuspension. In the experiments used by the previous authors, the particles are first deposited then resuspended. In reality, deposition and resuspension are simultaneous, and the available dust concentration on the ground is governed by resuspension, washout by runoff and absorption by soil water, production by deposition and other biological or mechanical processes. The detail of all these processes is essentially unknown, and we assume here that the available concentration of dust does only depend on the wetness of the surface. In this empirical view, the resuspension flux is governed by:

\[
F = Pf(w) u_*^{1.43}
\]  

(7.11)

where \( f(w) \) is a function of the soil water content and \( P \) is a constant tuned in order to approximately close the PM10 mass. The soil water modulation factor is vanishing for wet soil (gravimetric soil water content of 0.2 or more, as before, and is equal to 1 for dry soil, \( w \) less than 0.1). A linear relation is assumed between these values. The resuspension flux is found to be \( F=1800 \text{ mgm}^{-2}\text{h}^{-1} \) for a dry soil and for a friction velocity of 1 m.s\(^{-1}\). In Northern Europe the typical MM5 value for volumetric soil water content is 25%, and 0.5 m.s\(^{-1}\) for the friction velocity. This leads to a mass flux of about 170 \( \mu \text{g m}^{-2}\text{h}^{-1} \) and then about 1.4 ton.km\(^{-2}\) and per year, which is much larger than the anthropogenic emissions in most remote rural areas, but an order of magnitude smaller than that in urban areas. Finally, in the absence of any information the reentrained PM10 particle mass is supposed to be distributed in a standard atmospheric size distribution: 2/3 of the mass as PM2.5 and 1/3 as coarse PM1-PM2.5. Within PM2.5, particles are distributed as for the anthropogenic emissions.
Chapter 8

Initial and boundary conditions

8.1 Chemical boundary conditions

This section includes information for both initial and boundary conditions, both of which are treated in the same process although initial conditions extracted from a coarse scale simulation are only used for non-chained Chimere simulations.

8.1.1 Boundary conditions from global models

While some regional chemistry transport model rely on observation-based boundary concentrations, the Chimere strategy relies exclusively on simulations from global models. The added value in geographical and temporal variability as well as the larger number of chemical species available argue in favour of this second option, despite the increased sensitivity of the limited area CTM to any bias in the large scale forcing data. In order to cope with possible limitations in the global model forcing, we choose to increase the modularity of the global to regional nesting by allowing the use of several sources of boundary conditions (i.e. simulations from different models), or even combinations of such sources.

Three sources of boundary conditions were kindly made available by global chemistry-transport modelling groups to Chimere users. Their main characteristics are summarised below. The users are invited to take good care of acknowledging the work of their global modelling colleagues in their products and publications.

All the global fields provided for download are monthly climatologies (i.e. averages over several years for a given month of the year) but the code has the capacity to use time-varying boundary conditions if the user has such fields available (see section 8.1.4).

8.1.1.1 Available source of input data

MACC The global chemical reanalysis produced as part of the MACC II project (Monitoring Atmospheric Composition and Climat II, www.copernicus-atmosphere.eu) is also made available. The global MACC service provides a 5-yr reanalysis for the period 2004-2009 of trace gases and aerosol concentrations. A global monthly climatology at a resolution of 1.125° is made available to Chimere users. The MACC modelling system relies on the coupled IFS-Mozart [Horowitz, 2003] modelling and assimilation system for reactive gases and on the MACC prognostic aerosol module for particulate matter. Detailed validation of the MACC reanalysis can be found at: http://www.copernicus-atmosphere.eu/services/aqac/global_verification/validation_reports/.

For users, in case of publication using these MACC data, please add in your acknowledgements: This data set was provided by the MACC-II project, which is funded through the European Union Framework 7 programme. It is based on the MACC-II reanalysis for atmospheric composition; full access to and more information about this data can be obtained through the MACC-II web site (http://www.copernicus-atmosphere.eu).
The list of chemical species available in the MACC reanalysis is given in the list below.

- BC .................................... Black carbon
- BIGALK .................................. Lumped alkanes C>3
- BIGENE .................................. Lumped alkenes C>3
- C10H16 ................................ lumped monoterpenes
- C2H6 ..................................... Ethane
- CH2O ..................................... Formaldehyde
- CH3CHO ................................ Acetaldehyde
- CH4 ....................................... Methane
- CO ....................................... Carbon monoxide
- DUST1 ................ Desert dusts (0.03-0.55 µm)
- DUST2 ................ Desert dusts (0.55-0.9 µm)
- DUST3 ................ Desert dusts (0.9-20 µm)
- ALKAN .............................. Lumped alkanes C > 3
- AROM .............................. Lumped aromatics
- BC ........................................ Black carbon
- C2H4 ..................................... Ethylene
- C2H6 ..................................... Ethan
- C3H6 ..................................... Propen
- CH2O ..................................... Formaldehyde
- CH3CHO ................................ Acetaldehyde
- CH4 ....................................... Methane
- CNO3 ................................ Coarse Nitrate (2.5-5 µm)
- CO ....................................... Carbon monoxide
- DUST ...................................... Desert dusts (1-10 µm)
- GLYOXAL ............................ Glyoxal
- H2O2 ................................. Hydrogen peroxide
- HNO3 ................................. Nitric acid
- ISOP ..................................... Isoprene
- NH3 ...................................... Ammonia
- NO2 ......................................... Nitrogen dioxide
- O3 ......................................... Ozone
- PAN ...................................... Peroxy acetyl nitrate
- SO2 ......................................... Sulfur dioxide
- SO4 ......................................... Sulfate
- TOLUENE ................................ Toluene

**LMDDz-INCA** The historical and still commonly used set of boundary conditions is provided by the LMDz-INCA model (Laboratoire de Météorologie Dynamique General Circulation Model coupled with INCA: Interaction with Chemistry and Aerosols). The original INCA model is described in ([Hauglustaine et al., 2004] and [Folberth et al., 2006]) while developments related to aerosol modelling are presented in ([Bauer et al., 2004], [Schulz et al., 2006] and [Balkanski et al., 2007]). The specific version presented here is LMDz4-INCA3 with the nitrate chemistry introduced in [Hauglustaine et al., 2014]. It has 96x96 horizontal grid points and 19 vertical levels.

The list of chemical species available in the LMDz4-INCA3 model is given below. An example of surface mineral dust concentrations modelled with LMDz-INCA and MACC is presented in Figure 8.1.

- ALKAN .............................. Lumped alkanes C > 3
- AROM .............................. Lumped aromatics
- BC ........................................ Black carbon
- C2H4 ..................................... Ethylene
- C2H6 ..................................... Ethan
- C3H6 ..................................... Propen
- CH2O ..................................... Formaldehyde
- CH3CHO ................................ Acetaldehyde
- CH4 ....................................... Methane
- CNO3 ................................ Coarse Nitrate (2.5-5 µm)
- CO ....................................... Carbon monoxide
- DUST ...................................... Desert dusts (1-10 µm)
- H2O2 ................................. Hydrogen peroxide
- HNO3 ................................. Nitric acid
- NH3 ...................................... Ammonia
- NH4 ...................................... Particulate ammonium (0.1-1 µm)
- NO2 ......................................... Nitrogen dioxide
- NO3 ...................................... Particulate nitrate (0.1-1 µm)
- O3 ......................................... Ozone
- OC ....................................... Particulate organic carbon (0.1-1 µm)
- PAN ...................................... Peroxy acetyl nitrate
- SO2 ......................................... Sulfur dioxide
- SO4 ......................................... Sulfate

**GOCART** The Global model GOCART (NASA,[Ginoux et al., 2001]) was historically the only source of boundary conditions for particulate matter, it can still be used in combination with other sources for gaseous boundary conditions.

The list of chemical species available in the GOCART model is given in the list below. For each species, the size distribution is given in µm. An example of surface mineral dust concentrations modelled with GOCART and MACC is presented in Figure 8.2.

- DUST1 ................ Desert dusts (0.2-0.36)
- DUST2 ................ Desert dusts (0.36-0.6)
- DUST3 ................ Desert dusts (0.6-1.2)
- DUST4 ................ Desert dusts (1.2-2)
- DUST5 ................ Desert dusts (2-3.6)
- DUST6 ................ Desert dusts (3.6-6)
8.1.2 Structure of the boundary conditions from global models

All global forcing data are given in netcdf format with one file per month. Additional information on the input data are provided in the netcdf attributes for each variable. The most important attributes are "unit":

- **ppp** for part per part (mixing ratio),
- **ppb** for part per billion of 1e9 ppp,
- **ug** for micro-gram per cubic meter)

"typ" indicates if the variable is a gas ("gas"), desert dust ("dust") or non-dust aerosol ("aer"). The molar mass as used in the global model should also be provided.
In addition to concentration fields, the input files have latitude and longitude coordinates as well as the vertical grid (either 3D pressure on model levels or surface pressure + alpha and beta coefficients for the sigma-p grid). Would some conversion be required to provide concentrations in ppb to Chimere from the native unit in the global model (e.g. $\mu g m^{-3}$), the 3D temperature field is also requested in order to derive air density. Alternatively a constant and 3D uniform temperature of $15^\circ C$ is used.

The correspondence between the chemical species of the global model and Chimere is handled in the chemprep part of the code. This way, it is possible to use any source of input data for any of the chemical mechanism of Chimere.

The file **XXX_builder** (XXX is the name of a global concentrations dataset, GOCART, LMDZ-INCA or MACC at the moment) is used to build the interface between XXX and CHIMERE species. These files are split in 5 files types.

- For gas species: **XXX_builder.meca** where meca represents the chemical mechanism name (SAPRC/MELCHIOR1/MELCHIOR2)
- For SOA: **XXX_builder.aer.soa** where soa represents the SOA mechanism used (simple/medium/complex)
- For dust: **XXX_builder.dust** if the DUST specie are taken into account
- For primary aerosol species: **XXX.car** if the carbonaceous species are taken into account and ppmcarb if there are no carbonaceous species.
- For sea salts: **xxx_builder.nacl** if the sea salts are taken into account

Should any modification be added to the chemical scheme, these builders have to be modified accordingly. For example, the builder for LMDz-INCA and the SAPRC chemical mechanism is: **chemprep/boundaries_spec/INCAv2012_builder.saprc**

```bash
# Coarse species, typde, number of corresponding CHIMERE species,
# and for each species: name, molar mass, conversion factor
ALKAN gas 1 ALK3 59. 1.
AROM gas 1 ARO2 119. 1.
C2H4 gas 1 C2H4 28. 1.
C2H6 gas 1 ALK1 30. 1.
C3H6 gas 1 OLE1 72. 1.
CH2O gas 1 HCHO 30. 1.
CH3CHO gas 1 CH3CHO 44. 1.
CH4 gas 1 CH4 16. 1.
CO gas 1 CO 28. 1.
H2O2 gas 1 H2O2 34. 1.
```

Figure 8.2: *Surface mineral dust concentrations modelled with GOCART and LMDz-INCA for july.*
8.1.3 Adding new sources of input data

Basic netCDF manipulation using nco or cdo tools should allow advanced users to convert any global model fields into the appropriate format following the structure of the existing forcings and keeping one file per month, even if high frequency data are available. A new builder also needs to be written for each type of forcing. Apart from that, all the processing described in section 8.1.4, should work without distinction for any type of input data.

8.1.4 Boundary conditions interface

8.1.4.1 Chimere parameter file

In the chimere.par file, the user is invited to provide the path to its Boundary Conditions data (bcdir) together with a label pointing towards the relevant source (INCA, MACC, GOCART) as the name of the subdirectory where global data were extracted. The source of boundary data can be a composite of several global models for gas, dust and non-dust aerosol by using the right flags: bcfgas, bcdust, and bcaer. And for each of these flag the user can indicate whether climatological data (monthly means) are desired (with bcfgasdt, bcaerdta, or bcdustdt = 0), or if a higher temporal frequency is available (setting these flags to 1) in that case the fortran code extract automatically the highest available temporal resolution.

8.1.4.2 scripts/chimere-bound.sh

By reading the arguments in the chimere.par file, this script will link towards the right type of input data for each type of compound (gas, aer, dust). If several sources are required, the boundary condition extraction will be performed sequentially before being merged into a single file. In the case of time varying data, the script will try to locate the boundary conditions of the relevant years. Otherwise, for climatological data, the code looks for monthly data in the "clim" subdirectory. The boundary condition year is then handled as "0000".

8.1.4.3 src/prep/prep_bc.F90

The geometrical extraction as well as unit conversion is ultimately performed in the fortran part of the preprocessor. This code is generic an ignores the origin of the input data as long as the correct input format is provided. It can handle any temporal resolution of the boundary conditions and makes the difference between climatological and time-varying fields by checking whether the boundary condition year is "0000".

8.1.4.4 Output

The prep_bc.F90 program generates two groups of files: BOUN_CONCS.nc-* and INI_CONCS.nc-* . The files in each group are arranged by species types: gaseous ("-gas" suffix), aerosols ("-aer" suffix), and mineral dust ("-dust" suffix). prep_bc also generates the corresponding ASCII files with the ".lst" extension listing the actual *.nc files created by the program. The BOUN_CONCS.nc-* files contain trace species concentration on the outskirts of the Chimere domain for all the simulation time steps. The INI_CONCS.nc-* files contain initial conditions in the 3D limited-area domain; they are used if the model cannot find a previous Chimere run (see section 8.2).
8.1.5 Internal boundary conditions

Boundary conditions can be either "external" (see previous sections) or given by a coarse-resolution CHIMERE simulation. When a coarse-resolution simulation is available, i.e., when the `out.[coarse-label].nc` file exists, the `prep_chimere.F90` interface in the `src/prep` directory is used to generate the lateral and top boundary conditions to a nested run. This option is indicated by switching on the nest flag in `chimere.par`.

8.2 Initial concentrations

8.2.1 Initial concentrations species

There are two possible initialisation modes:

- Initialisation by reading initial concentrations in a restart file. This file must contain the "end" concentrations of a previous simulation, as provided in the `end.[label].nc` (and `exe.[label].nc` if the `pops` flag is activated). The species list is contained in the `end.[label].nc` file itself and is read by CHIMERE during initialisation.
- Initialisation by interpolating global concentration fields. This is the most common option used for a first initialisation.
- Initialisation by interpolating boundary conditions. Because of technical limitations, it is used only when the `pops` flag is activated (pops=1)

The top calling script checks the existence and non-emptiness of a file called `ini.[label].nc` (and `iex.[label].nc` if the `pops` flag is activated) in the simulation directory, which can be a copy of an "end" file. If it exists and is nonempty, then the initial conditions are used. In the other case, initial conditions are interpolated from boundary conditions. Initial conditions are read and put into arrays `conc` and `conco` in routine `src/initio/iniconc.F90`.

8.2.2 Initial concentrations interface

There are two types of initial conditions that can be used for CHIMERE: Initialized concentrations and non initialized concentrations. In the first case a file named `ini.[label].lst` is placed in the simulation directory (the same as where the CHIMERE output files `out.[label].nc`, `par.[label]`, and `end.[label]` are). In the second case there is no need to provide a file; initial conditions will be taken from interpolated global fields, layer by layer. The initial concentration files `INI_CONCS.nc-*` generated by `prep_bc.exe` are listed in the ASCII file `INI_CONCS.list`. When no restart files are available for the current run, the latter is linked to the initialisation file `ini.[label].lst` in the output directory. The `ini.[label].lst` file is used to initialise the simulation. When the restart file `end.[label].nc` from the previous simulation is available, it is linked to the `ini.[label].nc` file. This is automatically done in the `scripts/chimere-run1.sh` script. The format of the `ini.[label].nc` file is exactly the same as that of the `end.[label].nc` file. It contains the concentrations encoded in the netCDF format, described in Appendix G.7, p.175.

Initialisation is important for large-scale simulations (domains larger than about 500 Km × 500 km). Under extremely stagnant conditions, spin-up of one or two days may also be necessary at local (100 Km) scale. At regional scale, the spin-up time should be of the order of 4-5 days (for ozone and precursors).
Chapter 9

Meteorology

The meteorological data are used three different times in CHIMERE:

- §9.1: Input data: CHIMERE being an off-line model, input meteorological fields are necessary. These input data have to be reformatted to be read by CHIMERE.
- §9.2: Diagnostic parameters: Many meteorological parameters are required for a CHIMERE simulation. Depending on the input meteorological driver, they are not always available as input. Thus, in CHIMERE, a diagnostic program may be activated to parameterize the necessary but not provided parameters.
- §9.3: Transport and mixing: Once all meteorological data are available, they are used to mix and transport chemical species during the simulation.

9.1 Meteorological input data

CHIMERE is driven by meteorological fields from regional models, such as WRF or MM5 or global models such as ECMWF-IFS. To use these meteorological fields, available in various data format, CHIMERE contains several pre-processors to homogeneize these data and deliver a standard meteorological file to be read by the CHIMERE core: the NetCDF file `exdomout.nc`.

![Flow chart of the meteorological CHIMERE pre-processor.](image)

Figure 9.1: Flow chart of the meteorological CHIMERE pre-processor. WRF model is shown as an example of a weather forecast model driving CHIMERE. Programs are shown in yellow and NetCDF files in blue.

The top calling script of CHIMERE calls a program named `interf-[metname]` in the `meteo` directory. This program (usually a bourne shell script) has to be written by the user. One example is given: `interf-wrf` which is a generic interface to WRF. Figure 9.1 displays an example of
the pre-processor. The `prepwrf` interface takes a WRF output netcdf file `wrfout...` given by the `meteo_file` variable in `chimere.sh` and then by `fn_wrf` in `prepwrf.nml`. The list of WRF variables to process and their parameters are specified in the structure variable `varmeta` and are initialized in subroutine `initvars`. You might need to adjust this initialization (and the corresponding definitions of the parameters between `IFIRST` and `ILAST` in the beginning of the program), if your WRF output has variables additional to those specified in `varmeta`. The domain coordinate files `COORD_WRF`, `COORD_WRF_U`, and `COORD_WRF_V` are created by `prepwrf` from the WRF output netcdf files, so in contrast to MM5 you do not have to use an additional program for it. The `metdom` variable specified in `chimere.sh` is not used by the WRF interface.

This script `interf-wrf` calls a Fortran program, `prepwrf-interp.F90`. This program made several operations on the data:

- It transforms original meteorological variables given on the meteo model grid, at a frequency that is not necessarily one hour, to standard variables given on the CHIMERE horizontal grid as hourly values.
- The operations performed are horizontal and temporal interpolation, wind vector rotation, transformation from perturbation and mean values to the total ones, etc., depending on the original data format.
- Note there is no vertical interpolation (from the meteo file to CHIMERE) to conserve the full vertical resolution, for a better accuracy on turbulent diagnostics made later in CHIMERE (see §9.2)

At the end, a generic meteo file is created, `exdomout.nc`, with a dedicated CHIMERE format. In this file, some variables are mandatory, some others are optional. The file structure is entirely defined by the header listing in Appendix G.2, p.168. Table 9.1 lists these variables which must or can be output by the interpolation stage.

<table>
<thead>
<tr>
<th>File Name</th>
<th>Variable</th>
<th>Dimension</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mandatory Variables</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>lon</td>
<td>longitude of gridpoints</td>
<td>2D</td>
<td>degrees_east</td>
</tr>
<tr>
<td>lat</td>
<td>latitude of gridpoints</td>
<td>2D</td>
<td>degrees_north</td>
</tr>
<tr>
<td>alti</td>
<td>Altitude of half layer</td>
<td>3D</td>
<td>m</td>
</tr>
<tr>
<td>winz</td>
<td>Zonal component of the wind</td>
<td>3D</td>
<td>m/s</td>
</tr>
<tr>
<td>winm</td>
<td>Meridional component of the wind</td>
<td>3D</td>
<td>m/s</td>
</tr>
<tr>
<td>temp</td>
<td>Temperature</td>
<td>3D</td>
<td>K</td>
</tr>
<tr>
<td>sphu</td>
<td>Specific humidity</td>
<td>3D</td>
<td>kg/kg</td>
</tr>
<tr>
<td>pres</td>
<td>Pressure</td>
<td>3D</td>
<td>Pa</td>
</tr>
<tr>
<td>cliq</td>
<td>Cloud liquid water content (excluding rain water)</td>
<td>3D</td>
<td>Kg/Kg</td>
</tr>
<tr>
<td>swrd</td>
<td>Short Wave Radiation</td>
<td>2D</td>
<td>W/m²</td>
</tr>
<tr>
<td>lwrud</td>
<td>Long Wave Radiation</td>
<td>2D</td>
<td>W/m²</td>
</tr>
<tr>
<td>psfc</td>
<td>Surface pressure</td>
<td>2D</td>
<td>Pa</td>
</tr>
<tr>
<td>tem2</td>
<td>2m Temperature</td>
<td>2D</td>
<td>K</td>
</tr>
<tr>
<td>rh2m</td>
<td>2m Relative humidity</td>
<td>2D</td>
<td>0-1</td>
</tr>
<tr>
<td>weas</td>
<td>Water equiv. accum. snow depth</td>
<td>2D</td>
<td>mm</td>
</tr>
<tr>
<td>copc</td>
<td>Convective Precipitation</td>
<td>2D</td>
<td>kg/m²/hour</td>
</tr>
<tr>
<td>lspc</td>
<td>Large-scale Precipitation</td>
<td>2D</td>
<td>kg/m²/hour</td>
</tr>
<tr>
<td>Optional Variables</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>rain</td>
<td>rain water profile</td>
<td>3D</td>
<td>Kg/Kg</td>
</tr>
<tr>
<td>cice</td>
<td>ice profile</td>
<td>3D</td>
<td>Kg/Kg</td>
</tr>
<tr>
<td>sshf</td>
<td>Surface sensible heat flux</td>
<td>2D</td>
<td>W/m²</td>
</tr>
<tr>
<td>slhf</td>
<td>Surface latent heat flux</td>
<td>2D</td>
<td>W/m²</td>
</tr>
<tr>
<td>usta</td>
<td>Friction velocity</td>
<td>2D</td>
<td>m/s</td>
</tr>
<tr>
<td>hght</td>
<td>Boundary layer height</td>
<td>2D</td>
<td>m</td>
</tr>
<tr>
<td>lowc</td>
<td>Low cloud fraction</td>
<td>2D</td>
<td>m</td>
</tr>
<tr>
<td>medc</td>
<td>Medium cloud fraction</td>
<td>2D</td>
<td>m</td>
</tr>
<tr>
<td>higc</td>
<td>High cloud fraction</td>
<td>2D</td>
<td>m</td>
</tr>
</tbody>
</table>

Table 9.1: Mandatory and optional variables in `exdomout.nc` meteo file. Note that all meteorological 3D variables must be provided at half-layers levels.

The programs are provided for MM5, WRF and IFS/ECMWF. If other meteorological data have to be
used, the user should give it a name, [metname], and write the `interf-[metname]` bash program and the `prep[metname].F90` fortran program. The user should also change the "meteo=" line in the top calling script.

9.2 Diagnostics of parameters:

The second stage of the meteorological fields treatment is directly in the CHIMERE model, and during the hourly integration phase. Note that compared to the previous versions of CHIMERE, all these programs replace the `diagmet` programs. All programs are called by the `integr.run.F90` routine and are:

- `readmetro`: routine for the hourly reading of the `exdomout.nc` file
- `calc_turb`: calculation of turbulence on raw meteo profiles
- `calc_winw`: calculation of the vertical wind speed on chimere profiles
- `calc_deepconv`: calculation of deep convection fluxes (if required by the user)
- `checkcfl`: Estimation of the adaptative time-step
- `outprint`: Save meteo data (high vertical resolution) to the `meteo.$sim.nc` file.
- `met2chim`: Conversion of units from the meteo format to the specific CHIMERE format (molecules, centimeters and seconds).

9.2.1 Management of additional parameters

These calculations are done in the `calc_turb` routine. The first calculation is done to estimate several meteorological parameters, mandatory for CHIMERE but not always available with the meteorological input files. These parameters correspond to the optional parameters listed in Table 9.1. The calculations are done using the meteorological fields provided in the `exdomout.nc` file, i.e., already projected on the horizontal CHIMERE grid but still on the native meteo model vertical grid.

The availability of these parameters is checked during the reading of the `exdomout.nc` file. If the parameters exist, they are not recalculated, contrarily to the previous versions of CHIMERE where it was a user`s option. Indeed, we consider that if the variables exist, they correspond to recent parameterization in the meteorological model used and are consistent with other variables. They thus have to be keep.

If they are not available, the following parameters are diagnosed:

- If **boundary layer height** is not available from meteo data, it will be calculated. The boundary layer height is considered as the maximum of the [Troen and Mahrt, 1986] boundary layer height calculated from the Richardson number profile, as the lowest altitude where $R_i = 0.5$, and a more convectively-based boundary layer height calculation. The latter is based on a simplified and diagnostic version of the approach of [Cheinet and Teixeira, 2003]. It consists in the resolution of the (dry) thermal plume equation with diffusion. The in-plume vertical velocity and buoyancy equations are solved and the boundary layer is taken as the height where vertical velocity stops. Thermals are initiated with a non-vanishing vertical velocity and potential temperature departure, depending on the turbulence similarity parameters in the surface layer.

- The **friction velocity** $u^*$ is used for deposition and calculation of diffusivities. It is a particularly sensitive parameter for ozone in summer through the calculation of aerodynamic resistance $R_a$. It should strongly depend on land use type, which are critical to deposition. In meteorological models, especially large-scale, roughness lengths are sometimes estimated too roughly for the application to high-resolution deposition. The recalculation of $u^*$ which is proposed uses the [Louis et al., 1982] formulation which is particularly robust and gave satisfactory results.

- **Heat fluxes** are also used for the calculation of $w_a$ and therefore mixing, and the height of the boundary layer. In fact only the virtual heat flux is required, which can be recalculated from an empirical formula
Using temperatures in the first meteorological model layers. This formula is not very accurate.

- **The vertical turbulent diffusivity** $K_z$. Horizontal turbulent fluxes are not considered. Vertical turbulent mixing takes place only in the boundary-layer. The formulation uses K-diffusion following the parameterization of [Troen and Mahrt, 1986], without counter-gradient term. In each model column, diffusivity $K(z)$ is calculated as:

$$K_z = kw_s z \left(1 - \frac{z}{h}\right)^{1/3}$$  \hspace{1cm} (9.1)

where $w_s$ is a vertical scale given by similarity formulae.

- In the stable case (surface sensible heat flux < 0): $w_s = u_s/(1 + 4.7z/L)$
- In the unstable case: $w_s = (u_s^3 + 2.8ew_s^3)^{1/3}$

where $e = \max(0.1,z/h)$, $L$ is the Obukhov Length, $w_s$ is the convective velocity scale, $u_s$ the friction velocity and $h$ the boundary layer height. A minimal $K(z)$ is assumed, with a value of 0.01 $m^2/s$.

Finally, all three-dimensional meteorological fields are averaged over the CHIMERE vertical grid. Note that several fixed parameters are present in this `calc_turb` routine. They were chosen as the more realistic as possible and it is not recommended to modify these values. These constant values are listed in Table 9.2.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>pblmin</td>
<td>20.</td>
<td>Minimum PBL height</td>
</tr>
<tr>
<td>vkminup</td>
<td>0.1</td>
<td>Minimum $K_z$ above PBL (m$^2$/s)</td>
</tr>
<tr>
<td>z10m</td>
<td>10.</td>
<td>10 meters above ground level</td>
</tr>
<tr>
<td>soimdef</td>
<td>1.0</td>
<td>Default Soil Moisture (no resuspension/erosion)</td>
</tr>
<tr>
<td>woff</td>
<td>0.5</td>
<td>Wind offset to smooth Richardson numbers (m/s)</td>
</tr>
<tr>
<td>cthx</td>
<td>0.90</td>
<td>Min RH for cloud BLH enhancement</td>
</tr>
<tr>
<td>vymax</td>
<td>500.</td>
<td>Maximum $K_z$</td>
</tr>
<tr>
<td>odclw</td>
<td>0.18e3</td>
<td>Optical depth rate for liquid water</td>
</tr>
<tr>
<td>odic</td>
<td>0.06e3/0.9</td>
<td>Optical depth rate for ice</td>
</tr>
<tr>
<td>topcldmax</td>
<td>1000.</td>
<td>Maximum altitude of low clouds top</td>
</tr>
<tr>
<td>cloh</td>
<td>1</td>
<td>High cloud option for attenuation</td>
</tr>
<tr>
<td>crh2</td>
<td>0.95</td>
<td>High cloud option for attenuation</td>
</tr>
<tr>
<td>cloh2</td>
<td>0.005</td>
<td>High clouds optical depth /m for RH=1</td>
</tr>
<tr>
<td>ztherm</td>
<td>25.0</td>
<td>Height of thermals start</td>
</tr>
<tr>
<td>ric</td>
<td>0.5</td>
<td>Troen and Mahrt suggestion for critical Ri for BL top</td>
</tr>
<tr>
<td>dvsca</td>
<td>1000.0</td>
<td>Entrain./Detrain. first guess vertical scale (m)</td>
</tr>
<tr>
<td>vkmindry</td>
<td>0.01</td>
<td>Minimum $K_z$ in the dry boundary layer (m$^2$/s)</td>
</tr>
<tr>
<td>vkmindry</td>
<td>1.0</td>
<td>Minimum $K_z$ in cloudy boundary layer (m$^2$/s)</td>
</tr>
<tr>
<td>rlam</td>
<td>150.</td>
<td>Upper air mixing length</td>
</tr>
</tbody>
</table>

Table 9.2: Constant values used for the calculation of additional parameters in the routine `calc_turb`.

### 9.2.2 Estimation of the vertical velocity

This calculation is done in the `calc_winw` routine. The vertical velocity is diagnosed by using the horizontal fluxes. A simple momentum conservation relation is applied to calculate the vertical flux for the top of each model box (assuming that the first one, near the ground, is zero).

### 9.2.3 Deep convection fluxes

These calculations are done in the `calc_deepconv` routine. The calculation of deep convection fluxes is done only if the user defined the corresponding flag as ideepconv=1 in the `chimere.par` namelist file.
The deep convection scheme describes effects of subgrid scale clouds on tropospheric convection, after [Tiedtke, 1989]. Deep convection occurs when cumulus or cumulo-nimbus clouds (referred as convective clouds) are present. These clouds are formed when air masses are unstable, when warm air is at the surface or cold air is transported in upper layers (cold front). High vertical wind speed are observed leading to vertically extended cloud structures. On the other hand, when clouds are only due to mechanical forcings (mountains, warm fronts), they are named stratiform clouds and generally exhibit low vertical speed values.

Figure 9.2: [left] Temperatures changes due to shallow and deep convection and [right] Schematic view of a convective cloud

Air masses may be quickly mixed in the troposphere when convective unstabilities occured under a cloud. To describe this phenomenon, schemes generally consider a cloud (and the whole column including this cloud) and the environment. In the major part of deep convection parameterizations, the hypothesis of small cloud surface compared to the total studied surface is done. Under the cloud, updrafts and downdrafts are observed. The updraft originates from air masses lighter than their environment when downdrafts represent fall of colder air (often with rain). In the updraft and the downdraft, air may be exchange between the cloud and the environment: if air of environment flows to the cloud, this is the entrainment and if air of clouds flows towards environment, this is the detrainment. In order to ensure mass conservation, a compensatory subsidence is observed in the environment.

In CHIMERE, the Tiedtke scheme is implemented. The main goal of this scheme is to estimated a convection mass flux:

\[ M(z) = \rho(z)(a_{up}w_{up}(z) + a_{dw}w_{dw}(z)) = -\rho(z)a_{env}w_{env}(z) \] (9.2)

with \( w_{up}(z) > 0 \), \( w_{dw}(z) < 0 \) et \( w_{env}(z) < 0 \) the vertical wind speed in the updrafts, downdrafts and environment, respectively. The vertical gradient of this mass flux is:

\[ \frac{\partial M(z)}{\partial z}(z) = E(z) - D(z) \] (9.3)

with \( E(z) > 0 \) et \( D(z) > 0 \), the entrainment and detrainment fluxes. This equation works both for updrafts and downdrafts, with, for example for the updraft:

\[ E(z) = E_{up}(z) + E_{dw}(z) \] and \( D(z) = D_{up}(z) + D_{dw}(z) \) (9.4)

An example of estimated fluxes are displayed in the Figure 9.3.

These fluxes are used to estimates chemical concentrations fluxes as:
with the concentrations \(c_{\text{up}}, c_{\text{dw}}\) and \(c_{\text{env}}\) in the updraft, downdraft and environment, respectively. The parametrization is designed with the parameter names such as in the Figure 9.4.

The net flux is first estimated in the \texttt{locvalues.f90} routine. At this stage, the fluxes are in molecules.cm\(^{-2}\).s\(^{-1}\) (after conversion in \texttt{iniphys.f90}). For each grid cell, the Equation 9.3 is applied to give 'updraught mass flux' (flxuloc) and 'downdraught mass flux' (flxdloc). The calculation is done from surface to top domain in order to ensure mass conservation following the relation:

\[
FLXU(z) = \frac{\partial M_{\text{up}}(z)c_{\text{up}}(z)}{\partial z} = E_{\text{up}}(z)c_{\text{env}} - D_{\text{up}}(z)c_{\text{up}} + FLXU(z-1)
\]

\[
FLXD(z) = \frac{\partial M_{\text{dw}}(z)c_{\text{dw}}(z)}{\partial z} = E_{\text{dw}}(z)c_{\text{env}} - D_{\text{dw}}(z)c_{\text{dw}} + FLXD(z-1)
\]

The top level of the cloud and the detrainment (when \(E_{\text{dw}}(z) > 0\)) are estimated separately and names 'nvcloudtop' and 'nvdettop', respectively.

These fluxes are used in the \texttt{transmix.f90} routine. One have to note that the 'concu', 'cond' parameters are not concentrations but ratios of pollutants molecules number on air molecules number. This conversion is done to ensure 'trpr' and 'trlo' production and loss fluxes terms in molecule.cm\(^{-3}\).s\(^{-1}\). 'concu' and 'cond' are estimated using the mass conservation relation, as for example:

\[
FLXU(nv) \times \text{concu}(nv) = FLXU(nv-1) \times \text{concu}(nv-1) + dpeu(nv) \times \text{conc}(nv) - dpdu(nv) \times \text{concu}(nv)
\]

and we have:

\[
\text{concu}(nv) = \frac{FLXU(nv-1) \times \text{concu}(nv-1) + dpeu(nv) \times \text{conc}(nv)}{dpdu(nv) + FLXU(nv)}
\]
9.3 Transport and mixing

9.3.1 Horizontal transport

Three schemes for horizontal transport of chemical concentrations in the model are now available. The choice between the three may be done species by species by changing the second column flag in the ACTIVE_SPECIES file. The schemes are:

- A simple first-order upwind scheme named upwind in the model: low computational cost but not very accurate and very diffusive.
- The second-order Van Leer scheme: low computational cost and good accuracy for transport of high concentrations in plumes.
- The third-order PPM scheme (PPM stands for 'Parabolic Piecewise Method'), proposed by [Colella and Woodward, 1984]): high computational cost but more accurate for long-live species, naturally diffusive in a chemistry-transport model

These three schemes are all defined and used in the src/model/transmix.f90 program. We consider the following conservation equation:

$$\frac{\partial u}{\partial t} + \frac{\partial F_i(u)}{\partial x_i} = 0$$  \hspace{1cm} (9.10)$$

where $u = (\rho, \rho v_x, \rho v_y, \rho v_z, e)$ the physical conserved quantities (spatially) and $F(u)$ the corresponding flux. Each values and associated fluxes are represented at the center of each cell, $u_n = u(x_n)$; $F_n$. Of course, for a more realistic approach, we would represent these fluxes at each cells interface ($F_{n+1/2}$): thus, the problem of the advection schemes is to represent these interfaces fluxes by using only the known mean values fluxes. Formally, we can estimate the next time step $u$ with the following equation:
\[ u_n^{t+\Delta t} = u_n^{t+\Delta t} - \left( \frac{F_{n+1/2}^t - F_{n-1/2}^t}{\Delta x} \right) \Delta t \]  

(9.11)

This equation is exact because it ensures the mass conservation between inside and outside fluxes for each direction. To estimate the value of \( F_{n+1/2}^t \), we have to use the known values of \( F_n \) et \( F_{n+1} \). The way we use all these adjacent fluxes defines the "centered" or "advanced" scheme type and induces its numerical stability or not.

The following scheme is named "upwind" because it follows the advected flux. By the way, we choose the flux value we use as a function of the place we are and the direction we want to go, as:

\[ F_{n+1/2}^t = \begin{cases} 
F_n^t & \text{if } v > 0 \\
F_{n+1}^t & \text{if } v < 0 
\end{cases} \]  

(9.12)

This scheme is clearly asymmetrical. In addition, numerical experiments showed it is very diffusive. To avoid these effects, more complex schemes were developed: they are using more cells and thus are able to limit numerical errors due to too crude interpolations between cells. In the CHIMERE model, we implemented two advection schemes recognized for their good numerical accuracy: the VanLeer scheme in the src/model/vanleer.f90 program and the PPM scheme in the src/model/ppm.f90.

Horizontal mass fluxes (independent of species, first order) are calculated first at each coarse time step in routine src/model/htransport.f90, then the complete calculation using the species concentration and PPM is performed at each fine time step in routine src/model/transmix.f90.

### 9.3.2 Vertical transport

Vertical transport is assumed to balance horizontal mass divergence. Two schemes are implemented: the first-order upwind scheme and the second-order VanLeer scheme (NEW in chimere 2014b).

The vertical mass flux of dry air is calculated columnwise for each cell interface in the vertical direction, successively from model bottom to model top, in the following way:

- In the lowest layer, the lateral mass imbalance is calculated by summing up all the incoming mass fluxes at the lateral boundaries of the cell and subtracting the outgoing mass fluxes at lateral boundaries, the wind at the upper interface of the lowest model layer is then calculated in order to compensate this mass imbalance by an opposite flux at the cell’s upper boundary. This calculation is performed at the first order, assuming that the density of the air crossing a cell boundary is equal to the average density of the upstream cell, both for horizontal and vertical transport.

- The same calculation is then performed successively for each cell in all the column up to the model top, balancing the total imbalance of the mass flux from lateral and lower boundaries by an opposite mass flux at the upper boundary. These vertical transport mass fluxes (independent of species) are calculated first at each coarse time step in routine src/model/vtransport.f90.

The calculation of the concentration tendencies due to vertical transport for each model species is then performed at each fine time step in routine src/model/transmix.f90, performing first-order upwind vertical transport if parameter iadvv is set to 0 in chimere.par, and the second-order monotonous Van Leer I vertical transport scheme if iadvv is set to 1 in chimere.par. As the latter transport scheme needs two concentration values upstream of the considered boundary and one concentration value downstream, and this can not be secured next to model bottom and model top, CHIMERE switches back to upwind vertical transport for the cells where only one value of upstream concentration is available within the vertical simulation domain (including the boundary condition at model top).
9.3.3 Turbulent mixing

At each interface between layers \( k \) and \( k+1 \), one calculates an equivalent turbulent vertical velocity \( V_k \) and vertical mixing is expressed in layer \( k \) by the mass flux:

\[
\text{Net Flux} = V_k (C_{k+1} - C_k) / \Delta x_k,
\]

where \( C \) denotes concentrations, \( D \) densities and \( H \) layer thicknesses. Density ratios are applied since turbulent mixing must conserve mass in each model cell. An equivalent formula is used for the upper layer. The turbulent velocity \( V_k \) is deduced from \( K(z) \) using:

\[
V_k = \frac{K_z \Delta x_k}{\frac{1}{2}(H_k + H_{k+1})}
\] (9.13)

When the top of the boundary layer is above the model top, \( H_{k+1} \) is replaced by \( h - \text{<model-top>} \) in the previous equation.

The \( K(z) \) profile is calculated in routine src/model/mixing.f90, as well as the turbulent velocity profile. Vertical mixing mass fluxes (independent of species, first order) are calculated first at each coarse time step in routine src/model/vtransport.f90, then the complete calculation using the species concentration is performed at each fine time step in routine src/model/transmix.f90.
Chapter 10

Chemistry

10.1 The TWO-STEP time numerical solver

The numerical method for the temporal solution of the stiff system of partial differential equations is adapted from the second-order TWOSTEP algorithm originally proposed by [Verwer, 1994] for gas phase chemistry only. It is based on the application of a Gauss-Seidel iteration scheme to the 2-step implicit backward differentiation (BDF2) formula:

\[
c^{n+1} = \frac{4}{3}c^n - \frac{1}{3}c^{n-1} + \frac{2}{3}\Delta t R(c^{n+1}),
\]

with \( c^n \) being the vector of chemical concentrations at time \( t_n \), \( \Delta t \) the time step leading from time \( t_n \) to \( t_{n+1} \) and \( R(c) = \dot{c} = P(c) - L(c)c \) the temporal evolution of the concentrations due to chemical production and emissions (\( P \)) and chemical loss and deposition (\( L \)). Note that \( L \) is a diagonal matrix here. After rearranging and introducing the production and loss terms this equation reads

\[
c^{n+1} = \left(I + 2\frac{\Delta t}{3}L(c^{n+1})\right)^{-1}\left(\frac{4}{3}c^n - \frac{1}{3}c^{n-1} + \frac{2}{3}\Delta t P(c^{n+1})\right).
\]

The implicit nonlinear system obtained in this scheme can be solved pertinently with a Gauss-Seidel method (Verwer, 1994).

Figure 10.1: Principle of ‘operator-splitting’ versus Chimere integration

In CHIMERE the production and loss terms \( P \) and \( L \) in equation 10.2 are replaced by the modified terms
\( \dot{P} = P + P_h + P_v \) and \( \dot{L} = L + L_h + L_v \), respectively. \( P_h \) and \( P_v \) denote the temporal evolution of the concentrations due to horizontal (only advection) and vertical (advection and diffusion) inflow into the concerned grid box, \\( L_h \) and \( L_v \) the temporal evolution due to the respective outflow divided by the concentration itself. With this integration scheme, at each time step all physical and chemical processes are updated simultaneously. The "operator splitting" technique (see e.g. [McRae et al., 1982]), which is still a standard way of solving the 3D transport-chemistry-problem, and the associated "splitting error" are therefore avoided. Further advantages of the scheme are its stability even for quite long time steps due to the implicitness of the formulation and the simplicity of the code which facilitates the development of secondary models (adjoint, tangent linear) enormously.

In practice, time stepping has two time steps: a coarse time step, where all physical variables are calculated, and a fine step (refined step in order to gain accuracy on chemistry). During loops over fine steps, physical variables are maintained constant.

In the provided version for the continental models, we chose a "very quick formulation", with a 10-minute physical step, no sub-chemical steps, i.e. all processes are stepped to 10 minutes, with only 1 Gauss-Seidel iteration. It is STRONGLY recommended, in order to have more accurate results, to use 2 Gauss-Seidel iterations, which increases by 2 the computer time. This change affects mostly concentrations during morning. However, for values of ozone concentration, the proposed version does not appear to degrade simulations, especially during afternoon hours.

The TWOSTEP formulae and loops are performed in module src/model/twostep_mod.f90.

10.2 Gas-phase chemistry

10.2.1 Chemical mechanisms (gas phase)

CHIMERE offers the option to include different gas phase chemical mechanisms. The original, complete scheme ([Lattuati, 1997]), hereafter called MELCHIOR1, describes more than 300 reactions of 80 gaseous species. The hydrocarbon degradation is fairly similar to the EMEP gas phase mechanism ([Simpson, 1992]). Adaptations are made in particular for low NOx conditions and NOx-nitrate chemistry. All rate constants are updated according to [Atkinson et al., 1997] and [De Moore et al., 1994]. Heterogeneous formation of HONO from deposition of NO2 on wet surfaces is now considered, using the formulation of [Aumont et al., 2003]. In order to reduce the computing time a reduced mechanism with less than species and about 120 reactions is derived from MELCHIOR ([Derognat et al., 2003]), following the concept of "chemical operators" ([Carter, 1990]). This reduced mechanism is called MELCHIOR2 hereafter. A third gas phase chemical mechanism is now available: SAPRC-07-A ([Carter, 2010], http://www.engr.ucr.edu/~carter/SAPRC/). It describes more than 275 reactions of 85 species and it is the most recent mechanism of mechanisms proposed in CHIMERE.

The base chemical mechanisms files are placed in chemprep/data, the mecanisms are automatically generated and placed in the chemprep/inputdata directories. New mechanisms can be implemented, in this case a work on the chemprep/chemprep.awk is required in adequation with the REACTIONS file for a new set of reactions. Not all forms of reactions are allowed. Arrhenius, Troe, photolysis and few other classical reaction rate types are only allowed. Introducing other types implies some recoding. See the technical documentation (the chemprep preprocessor). A file with altitude-dependent photolysis rates must also be provided, named PHOTO_PARAMETERS.[meca] in chemprep/data. Photolysis rates are calculated under clear sky conditions as a function of height using the TUV model ([Madronich et al., 1998]). Then clouds are taken into account in a highly parameterized fashion.

**Important notice:** Photolysis rates are estimated only up to 13000m. If you want to use the model with higher vertical levels, you have to remember CHIMERE results would be correct for transport (with \( z_{\text{max}}=14\ 000\text{m} \)) but NOT for gas chemistry.
Gas-phase chemistry constants is read in initialization routine src/initio/inichem.f90. Then rates are calculated at the coarse time step in routine src/model/rates.f90, but chemical fluxes are calculated for all species at the fine time step in routine src/model/chemistry.f90.

10.2.2 Species list of the reduced MELCHIOR1 gas-phase chemical mechanism

<table>
<thead>
<tr>
<th>Species</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Inorganic compounds</strong></td>
<td></td>
</tr>
<tr>
<td>O₃</td>
<td>ozone</td>
</tr>
<tr>
<td>H₂O₂</td>
<td>hydrogen peroxide</td>
</tr>
<tr>
<td>OH</td>
<td>hydroxyl radical</td>
</tr>
<tr>
<td>HO₂</td>
<td>hydroperoxy radical</td>
</tr>
<tr>
<td>NO</td>
<td>nitric oxide</td>
</tr>
<tr>
<td>NO₂</td>
<td>nitrogen dioxide</td>
</tr>
<tr>
<td>NO₃</td>
<td>nitrogen trioxide</td>
</tr>
<tr>
<td>N₂O₅</td>
<td>dinitrogen pentoxide</td>
</tr>
<tr>
<td>HONO</td>
<td>nitrous acid</td>
</tr>
<tr>
<td>HNO₃</td>
<td>nitric acid</td>
</tr>
<tr>
<td>HNO₄</td>
<td>pernitric acid</td>
</tr>
<tr>
<td>CO</td>
<td>carbon monoxide</td>
</tr>
<tr>
<td>SO₂</td>
<td>sulfur dioxide</td>
</tr>
<tr>
<td>H₂SO₄</td>
<td>sulfuric acid</td>
</tr>
<tr>
<td><strong>Hydrocarbon species</strong></td>
<td></td>
</tr>
<tr>
<td>C₄H₈</td>
<td>isoprene</td>
</tr>
<tr>
<td>OXYL</td>
<td>o-xylene</td>
</tr>
<tr>
<td>C₂H₄</td>
<td>ethene</td>
</tr>
<tr>
<td>C₂H₂</td>
<td>propene</td>
</tr>
<tr>
<td>C₃H₆</td>
<td>ethene</td>
</tr>
<tr>
<td>C₅H₈</td>
<td>isoprene</td>
</tr>
<tr>
<td>APINEN</td>
<td>α-pinene</td>
</tr>
<tr>
<td>BPINEN</td>
<td>β-pinene</td>
</tr>
<tr>
<td>LIMONE</td>
<td>limonene</td>
</tr>
<tr>
<td>TERPEN</td>
<td>terpenes (lumped class)</td>
</tr>
<tr>
<td>HUMULE</td>
<td>Humulene (lumped class)</td>
</tr>
<tr>
<td>OCIMEN</td>
<td>Ocimene (lumped class)</td>
</tr>
<tr>
<td><strong>Alcohol species</strong></td>
<td></td>
</tr>
<tr>
<td>C₂H₅OH</td>
<td>ethanol</td>
</tr>
<tr>
<td>C₃H₇OH</td>
<td>methanol</td>
</tr>
<tr>
<td><strong>Carbonyls</strong></td>
<td></td>
</tr>
<tr>
<td>HCHO</td>
<td>formaldehyde</td>
</tr>
<tr>
<td>CH₃CHO</td>
<td>acetaldehyde</td>
</tr>
<tr>
<td>CH₃COE</td>
<td>methyl ethyl ketone</td>
</tr>
<tr>
<td>CH₃COY</td>
<td>dimethyl glyoxal</td>
</tr>
<tr>
<td>MEMALD</td>
<td>4-oxo-2-pentenal</td>
</tr>
<tr>
<td>MAC</td>
<td>methacroleine</td>
</tr>
<tr>
<td>MVK</td>
<td>vinyl ketone</td>
</tr>
<tr>
<td>GLYOX</td>
<td>glyoxal</td>
</tr>
<tr>
<td>MGLYOX</td>
<td>methyl glyoxal</td>
</tr>
<tr>
<td>OFURAN</td>
<td>5-methyl-3H-furan-2-one</td>
</tr>
<tr>
<td><strong>Organic nitrates</strong></td>
<td></td>
</tr>
<tr>
<td>CH₃NO₃</td>
<td>methyl nitrate</td>
</tr>
<tr>
<td>ETNO₃</td>
<td>ethyl nitrate</td>
</tr>
<tr>
<td>BUNO₃</td>
<td>n-butyl-2-nitrate</td>
</tr>
<tr>
<td>ISNI</td>
<td>unsaturated nitrate from RO2P1</td>
</tr>
<tr>
<td>CARNIT</td>
<td>nitrate carbonyl taken as α-nitrooxy acetone</td>
</tr>
<tr>
<td>ORNIT1</td>
<td>α-hydroperox nitrate</td>
</tr>
<tr>
<td>ORNIT2</td>
<td>α-hydroperox nitrate from C₅H₈ and APINEN</td>
</tr>
<tr>
<td><strong>Peroxy radicals</strong></td>
<td></td>
</tr>
<tr>
<td>C₂H₅O₂</td>
<td>peroxy ethyl</td>
</tr>
<tr>
<td>C₂H₅O₂C</td>
<td>ethyl hydroperoxy</td>
</tr>
<tr>
<td>C₃H₇O₂</td>
<td>methyl peroxy</td>
</tr>
<tr>
<td>C₃H₇COO</td>
<td>peroxy acetyl radical</td>
</tr>
<tr>
<td>C₃H₇HX</td>
<td>propyl hydroperoxy</td>
</tr>
<tr>
<td>C₃H₇COX</td>
<td>peroxy from butan-2-one</td>
</tr>
<tr>
<td>C₃H₇COZ</td>
<td>peroxy from MACO₂+OH reaction</td>
</tr>
<tr>
<td>SECCBUO</td>
<td>2-oxo butyl</td>
</tr>
<tr>
<td>SECC₄H</td>
<td>peroxy butylin</td>
</tr>
<tr>
<td>OXYL₁</td>
<td>peroxy radical from OXYL</td>
</tr>
<tr>
<td>RO₂IP₁</td>
<td>peroxy radical from C₅H₈+OH reaction</td>
</tr>
<tr>
<td>MEMAL₁</td>
<td>peroxy radical from OH on MEMALD</td>
</tr>
<tr>
<td>MEMAL₂</td>
<td>peroxy radical from abstraction of OH in alpha position</td>
</tr>
<tr>
<td>MACO₂</td>
<td>peroxy radical from MAC+OH reaction</td>
</tr>
<tr>
<td>MVKO₂</td>
<td>peroxy radical from MVK</td>
</tr>
<tr>
<td>APIOH</td>
<td>Peroxy radical from APIEN+OH reaction</td>
</tr>
<tr>
<td><strong>Peroxy nitrates</strong></td>
<td></td>
</tr>
<tr>
<td>RNC₄H₄</td>
<td>peroxy ethyl nitrate</td>
</tr>
<tr>
<td>RNC₃H₆</td>
<td>peroxy propyl nitrate</td>
</tr>
<tr>
<td>RNC₅H₈</td>
<td>peroxy from C₅H₈+NO₃ reaction</td>
</tr>
<tr>
<td>ROXYL₁</td>
<td>peroxy from OXYL+NO₃ reaction</td>
</tr>
<tr>
<td>ISNIRO</td>
<td>peroxy from ISNI+OH reaction</td>
</tr>
<tr>
<td>APINO₃</td>
<td>Peroxy radical from APINEN+NO₃ reaction</td>
</tr>
<tr>
<td><strong>Pernitrates</strong></td>
<td></td>
</tr>
<tr>
<td>PAN</td>
<td>peroxy acetyl nitrate</td>
</tr>
</tbody>
</table>
| MACPAN          | peroxy acyl nitrate from MAC####
| CH₃NO₄          | methyl peroxy                                   |
| MEMPAN          | peroxy acyl nitrate from MEMAL2                |
| **Peroxide**    |                                                  |
| APIO₂H          | hydroperoxo from APINENO₃+HO₂ reaction          |
| BUO₂H           | Butyl hydroperoxide                             |
| CH₃O₂C          | hydroxethyl hydroperoxide                       |
| CH₃O₂H          | methyl hydroperoxide                            |
| CH₄CHX          | hydroxypropyl hydroperoxide                     |
| CH₄COX          | butan-2-one-3-hydroperoxide                     |
| CH₄COZ          | hydroperoxo from CH₃COZ+HO₂ reaction            |
| ET₀₂H           | ethyl hydroperoxide                             |
| MAC₀₂H           | hydroperoxo from MAC₀₂+HO₂ reaction            |
| MEMAH₂          | hydroperoxo from MEMAL₂+HO₂ reaction           |
| MEMAL₉           | hydroperoxo from MEMAL₁+HO₂ reaction           |
| MVKO₂H           | hydroperoxo from MVKO₂+HO₂ reaction            |
| OXYL₁H           | hydroperoxo from OXYL₁+HO₂ reaction            |
| PEROX           | hydroperoxo from RO₂P₁+HO₂ reaction            |
| PPA             | peroxy acetyl acid                              |

¹Hydrocarbon model species (except for CH₄ and C₂H₄) represent groups of hydrocarbons with similar reactivity. As “definition” a typical representative of this group is given. This is also true for the degradation products.
## Reaction list of the reduced MELCHIOR1 chemical mechanism

### Inorganic

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Kinetic constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>O₃+NO → NO₂</td>
<td>k(T)=Ae⁻⁸₂/T, A=1.8⁻¹², B=1370</td>
</tr>
<tr>
<td>O₃+NO₂ → NO₃</td>
<td>k(T)=Ae⁻²²⁻¹⁵/T, A=3.2⁻¹², B=2450</td>
</tr>
<tr>
<td>O₃+HO → HO₂</td>
<td>k(T)=Ae⁻⁸₂⁻¹⁵/T, A=1.9⁻¹², B=1000</td>
</tr>
<tr>
<td>NO+HO₂ → OH</td>
<td>k(T)=Ae⁻²²⁻¹⁵/T, A=1.4⁻¹⁴, B=600</td>
</tr>
<tr>
<td>NO₂+OH → NO₃</td>
<td>k(T)=Ae⁻²₂⁻¹⁵/T, A=2.9⁻¹², B=250</td>
</tr>
<tr>
<td>NO₃+HO → NO₂</td>
<td>k(T)=Ae⁻²₂⁻¹⁵/T, A=7.2⁻¹², B=785</td>
</tr>
<tr>
<td>HO₂+OH → H₂O</td>
<td>k(T)=Ae⁻⁸₂⁻¹⁵/T, A=4.8⁻¹¹, B=250</td>
</tr>
<tr>
<td>H₂O₂+OH → HO₂</td>
<td>k(T)=Ae⁻²²⁻¹⁵/T, A=2.9⁻¹², B=160</td>
</tr>
<tr>
<td>HNO₃+OH → NO₃</td>
<td>k(T)=Ae⁻²₂⁻¹⁵/T, A=2.3⁻¹⁵, B=3200</td>
</tr>
<tr>
<td>NO₂+HO₂ → OH</td>
<td>k(T)=Ae⁻²₂⁻¹⁵/T, A=4⁻¹⁰, B=12</td>
</tr>
<tr>
<td>HO₂+NO₂ → NO₃</td>
<td>k(T)=Ae⁻²₂⁻¹⁵/T, A=1.8⁻¹², B=90, N=1</td>
</tr>
</tbody>
</table>

### SOₓ

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Kinetic constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>SO₂+CH₃O₂ → H₂SO₄+HCHO+HO₂</td>
<td>k=4⁻²⁰</td>
</tr>
<tr>
<td>SO₂+OH+M → H₂SO₄+H₂O₂</td>
<td>k(T,M)=troe(4⁻¹⁰⁻¹⁵, 0, 3.3⁻¹⁰⁻¹⁵, 2⁻¹⁰⁻¹⁵, 0, 0.0⁻¹⁰⁻¹⁵)</td>
</tr>
</tbody>
</table>

### OH

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Kinetic constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH₄+OH → CH₃O₂</td>
<td>k(T)=Ae⁻²²⁻¹⁵/T, A=2.3⁻¹², B=1765</td>
</tr>
<tr>
<td>C₂H₆+OH → C₂H₅O₂</td>
<td>k(T)=Ae⁻²²⁻¹⁵/T, A=7.9⁻¹², B=1030</td>
</tr>
<tr>
<td>C₂H₄+OH+M → CH₂O₂C</td>
<td>k(T,M)=troe(7⁻¹⁰⁻¹⁵, 0, 3.1⁻¹⁰⁻¹⁵, 1⁻¹⁰⁻¹⁵, 0, 0.0⁻¹⁰⁻¹⁵)</td>
</tr>
<tr>
<td>CH₃O+OH → CH₃O₂</td>
<td>k(T)=Ae⁻²²⁻¹⁵/T, A=7.2⁻¹², B=360</td>
</tr>
<tr>
<td>CH₂H₂O+OH → CH₃CHOX</td>
<td>k(T)=Ae⁻²²⁻¹⁵/T, A=1.4⁻¹², B=20</td>
</tr>
</tbody>
</table>

### OMV

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Kinetic constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>HCHO+OH → CO+HO₂</td>
<td>k(T)=Ae⁻²²⁻¹⁵/T, A=8.6⁻¹², B=20</td>
</tr>
<tr>
<td>CH₃CHO+OH → CH₃COO</td>
<td>k(T)=Ae⁻²²⁻¹⁵/T, A=5.6⁻¹², B=310</td>
</tr>
<tr>
<td>CH₃CO+OH → CH₃COX</td>
<td>k(T)=Ae⁻²²⁻¹⁵/T, A=2.9⁻¹², B=414, N=2</td>
</tr>
<tr>
<td>MEMALD+OH → MEMAL1</td>
<td>k=5.6⁻¹¹</td>
</tr>
<tr>
<td>GLYOX+OH → 2*CO+HO₂</td>
<td>k=1.1⁻¹¹</td>
</tr>
<tr>
<td>MGLYOX+OH → CH₃COO+CO</td>
<td>k=1.5⁻¹¹</td>
</tr>
<tr>
<td>OFURAN+OH → MVKO₂</td>
<td>k=6.9⁻¹¹</td>
</tr>
<tr>
<td>MAC+OH → 0.5*MACO₂</td>
<td>k(T)=Ae⁻²²⁻¹⁵/T, A=1.8⁻¹², B=175</td>
</tr>
<tr>
<td>MVK+OH → MVKO₂</td>
<td>k(T)=Ae⁻²²⁻¹⁵/T, A=4.1⁻¹², B=453</td>
</tr>
<tr>
<td>CH₃O₂H+OH → CH₃O₂</td>
<td>k(T)=Ae⁻²²⁻¹⁵/T, A=1.9⁻¹², B=190</td>
</tr>
</tbody>
</table>
Reactions | Kinetic constants
--- | ---
ETO2H+OH → C2H5O2 | k(T)=Ae^{-B/T}, A=1.9×10^{-12}, B=190
PPA+OH → CH3COO | k(T)=Ae^{-B/T}, A=1.9×10^{-12}, B=190
BUO2H+OH → SECC4H | k(T)=Ae^{-B/T}, A=1.9×10^{-12}, B=190
CH4COX+OH → CH3COX | k(T)=Ae^{-B/T}, A=1.9×10^{-12}, B=190
CH3O2C+OH → CH2O2C | k(T)=Ae^{-B/T}, A=1.9×10^{-12}, B=190
CH4CHX+OH → CH3CHX | k(T)=Ae^{-B/T}, A=1.9×10^{-12}, B=190
OXYLH1+OH → OXYL1 | k(T)=Ae^{-B/T}, A=1.9×10^{-12}, B=190
MEMALH+OH → MEMAL1 | k(T)=Ae^{-B/T}, A=1.9×10^{-12}, B=190
MEMAH2+OH → MEMAL2 | k(T)=Ae^{-B/T}, A=1.9×10^{-12}, B=190
PEROX+OH → RO2IP1 | k(T)=Ae^{-B/T}, A=1.9×10^{-12}, B=190
MACO2H+OH → MACO2 | k(T)=Ae^{-B/T}, A=1.9×10^{-12}, B=190
MEMAL2+OH → MEMAL1 | k(T)=Ae^{-B/T}, A=1.9×10^{-12}, B=190
MEMAH2+OH → MEMAL2 | k(T)=Ae^{-B/T}, A=1.9×10^{-12}, B=190
MACO2H+OH → MACO2 | k(T)=Ae^{-B/T}, A=1.9×10^{-12}, B=190
MEMAH2+OH → MEMAL2 | k(T)=Ae^{-B/T}, A=1.9×10^{-12}, B=190
MEMALH+OH → MEMAL1 | k(T)=Ae^{-B/T}, A=1.9×10^{-12}, B=190
CH3O2H+OH → HCHO+OH | k(T)=Ae^{-B/T}, A=1.9×10^{-12}, B=190
ETO2H+OH → CH3CHO+OH | k(T)=Ae^{-B/T}(300/T)^N, A=1.30×10^{-13}, B=-1176, N=-2
BUO2H+OH → CH3COE+OH | k(T)=Ae^{-B/T}(300/T)^N, A=6.1×10^{-14}, B=-1681, N=-2
CH4COX+OH → CH3COY+OH | k(T)=Ae^{-B/T}(300/T)^N, A=6.1×10^{-14}, B=-1533, N=-2
CH3O2C+OH → 2HCHO+OH | k(T)=Ae^{-B/T}(300/T)^N, A=6.1×10^{-14}, B=-1238, N=-2
CH3O2C+OH → 2HCHO+OH | k(T)=Ae^{-B/T}(300/T)^N, A=4.05×10^{-13}, B=-688, N=-2
CH4CHX+OH → HCHO+CH3CHO+OH | k(T)=Ae^{-B/T}(300/T)^N, A=4.05×10^{-13}, B=-688, N=-2
OXYLH1+OH → MEMALD+MGLYOX+OH | k(T)=Ae^{-B/T}(300/T)^N, A=1.44×10^{-14}, B=-1403, N=-2
MEMALH+OH → GLYOX+MGLYOX+OH | k(T)=Ae^{-B/T}(300/T)^N, A=1.27×10^{-13}, B=-1403, N=-2
MEMAH2+OH → MALEIC+CH3O2 | k(T)=Ae^{-B/T}(300/T)^N, A=6.1×10^{-14}, B=-1681, N=-2
MACO2H+OH → CH3COZ | k(T)=Ae^{-B/T}, A=1.91×10^{-13}, B=-1193, N=-2
APIO2H+OH → CH3CHO+CH3COE+OH | k(T)=Ae^{-B/T}(300/T)^N, A=3.82×10^{-13}, B=-882, N=-2
NO3

CH4+NO3 → CH3O2+HNO3 | k=4×10^{-5}
C2H6+NO3 → C2H5O2+HNO3 | k=8×10^{-8}
NC4H10+NO3 → SECC4H+HNO3 | k=5×10^{-5}
C2H4+NO3 → RNC2H4 | k=2×10^{-6}
C3H6+NO3 → RNC3H6 | k=9.45×10^{-15}
OXYL+NO3 → ROXYL1+HNO3 | k=3.7×10^{-16}
CH3OH+NO3 → CH3O2+HNO3 | k=7.8×10^{-13}
C2H5OH+NO3 → C2H5O2+HNO3 | k=9×10^{-16}
HCHO+NO3 → CH3O2+HNO3 | k=5×10^{-16}
CH3CHO+NO3 → CH3COO+HNO3 | k=8×10^{-15}
CH3O2+NO3 → CH3O+H3O3 | k=1×10^{-12}
C2H5O2+NO3 → C2H5O2+H2O2 | k=1×10^{-12}
CH3COO+NO3 → CH3O2+NO2+CO2 | k=4×10^{-12}
CH2O2C+NO3 → CH2O2C+H2O2 | k=1×10^{-12}
SECC4H+NO3 → SECBUO+H2O2 | k=1×10^{-12}
CH3COX+NO3 → CH3COY+NO2+H2O | k=1×10^{-12}
CH3CHX+NO3 → CH3CHO+HNO3+NO2+H2O | k=1×10^{-12}
OXYL1+NO3 → MEMALD+MGLYOX+NO2+H2O | k=1×10^{-12}
MEMAL1+NO3 → GLYOX+MGLYOX+NO2+H2O | k=1×10^{-12}
MEMAL2+NO3 → MALEIC+NO2+CH3O2 | k=4×10^{-12}
MACO2+NO3 → CH3COZ+NO2+CO2 | k=4×10^{-12}
<table>
<thead>
<tr>
<th>Reactions</th>
<th>Kinetic constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>RO2IP1+NO3—0.38<em>MAC+0.50</em>MVK+0.88<em>HCHO+0.12</em>RO2IP1+0.88*HO2+NO2</td>
<td>k=1.2e-12</td>
</tr>
<tr>
<td>MVK02+NO3—0.28<em>MGLYOX+0.28</em>HCHO+0.72<em>CH3CHO+0.72</em>CH3COO+0.28*HO2+NO2</td>
<td>k=1.2e-12</td>
</tr>
<tr>
<td>CH3COZ+NO3—CH3COE+HO2+NO2</td>
<td>k=1.2e-12</td>
</tr>
<tr>
<td>APIOH+NO3—CH3CHO+CH3COE+NO2+HO2</td>
<td>k=1.2e-12</td>
</tr>
<tr>
<td>RNC2H4+NO3—0.5<em>CARNIT+HCHO+1.5</em>NO2+0.5*HO2</td>
<td>k=1.2e-12</td>
</tr>
<tr>
<td>RNC3H6+NO3—0.5<em>CARNIT+0.5</em>CH3CHO+0.5<em>HCHO+1.5</em>NO2+0.5*HO2</td>
<td>k=1.2e-12</td>
</tr>
<tr>
<td>ROXYL1+NO3—BENZAL+NO2+HO2</td>
<td>k=1.2e-12</td>
</tr>
<tr>
<td>ISNIR+NO3—0.95<em>CH3CHO+0.475</em>MGLYOX+0.05<em>ISNI+0.05</em>HO2+1.9*NO2</td>
<td>k=1.2e-12</td>
</tr>
<tr>
<td>RNC5H8+NO3—0.85<em>ISNI+0.1</em>MAC+0.05<em>MVK+0.15</em>HCHO+1.1<em>NO2+0.8</em>HO2</td>
<td>k=1.2e-12</td>
</tr>
<tr>
<td>APINO3+NO3—CH3CHO+CH3COE+2*NO2</td>
<td>k=1.2e-12</td>
</tr>
<tr>
<td>O3</td>
<td>^B^/T \cdot A=9.1e-15,B=2580</td>
</tr>
<tr>
<td>C2H4+O3—HCHO+0.12<em>HO2+0.13</em>H2+0.44*CO</td>
<td>k(T)=^B^/T \cdot A=5.5e-15,B=1880</td>
</tr>
<tr>
<td>C3H6+O3—0.53<em>HCHO+0.5</em>CH3CHO+0.31<em>CH3O2+0.28</em>HO2+0.15<em>OH+0.45</em>CO+0.7*CH4</td>
<td>k(T)=^B^/T \cdot A=1.2e-14,B=2013</td>
</tr>
<tr>
<td>C5H8+O3—MAC+0.3<em>HCHO+0.25</em>CH3CHO+0.25<em>CH3O2+0.25</em>CH3COO+0.05<em>ISNI+0.05</em>HO2+1.9*NO2</td>
<td>k(T)=^B^/T \cdot A=5.3e-15,B=2520</td>
</tr>
<tr>
<td>MAC+O3—0.8<em>MGLYOX+0.7</em>HCHO+0.25<em>CH3CHO+0.25</em>CH3O2+0.25<em>CH3COO+0.25</em>ISNI+0.25*HO2</td>
<td>k(T)=^B^/T \cdot A=4.3e-15,B=2520</td>
</tr>
<tr>
<td>MVK+O3—0.82<em>MGLYOX+0.8</em>HCHO+0.04<em>CH3CHO+0.04</em>CH3O2+0.04<em>CH3COO+0.04</em>CH3COE+0.04*ISNI</td>
<td>k=6e-18</td>
</tr>
<tr>
<td>PEROX+O3—0.7*HCHO</td>
<td>k=6e-18</td>
</tr>
<tr>
<td>organic</td>
<td></td>
</tr>
<tr>
<td>CH3O2+NO—HCHO+NO2+HO2</td>
<td>k(T)=^B^/T \cdot A=4.2e-12,B=-180</td>
</tr>
<tr>
<td>C2H5O2+NO—CH3CHO+NO2+H2O</td>
<td>k=8.7e-12</td>
</tr>
<tr>
<td>CH3COO+NO—CH3O2+NO2+CO2</td>
<td>k=2e-11</td>
</tr>
<tr>
<td>CH2O2C+NO—2*HCHO+NO2+H2O</td>
<td>k=9e-12</td>
</tr>
<tr>
<td>SECC4H+NO—SECCBUO+NO2</td>
<td>k=4e-12</td>
</tr>
<tr>
<td>SECC4H+NO+M—SECCBUO+NO2</td>
<td>k(T,M)=troe(-3.76e-32,0,0,-3.3e-12,0,8.1,0.41)</td>
</tr>
<tr>
<td>SECBUO+M—CH3COE+HO2</td>
<td>k(T)=^B^/T \cdot A=3.0e-14,B=200</td>
</tr>
<tr>
<td>SECBUO—CH3CHO+CH5H2O</td>
<td>k(T)=^B^/T \cdot A=7.20e+12,B=5780</td>
</tr>
<tr>
<td>CH3COX+NO—CH3COY+NO2+H2O</td>
<td>k=4e-12</td>
</tr>
<tr>
<td>CH3CHX+NO—HCHO+CH3CHO+NO2+H2O</td>
<td>k=4e-12</td>
</tr>
<tr>
<td>OXYL1+NO—MEMALD+MGLYOX+NO2+H2O</td>
<td>k=4e-12</td>
</tr>
<tr>
<td>MEMAL1+NO—GLYOX+MGLYOX+NO2+H2O</td>
<td>k=4e-12</td>
</tr>
<tr>
<td>MEMAL2+NO—MALEIC+NO2+CH3O2</td>
<td>k=4e-12</td>
</tr>
<tr>
<td>MACO2+NO—CH3COZ+NO2+CO2</td>
<td>k=4e-12</td>
</tr>
<tr>
<td>RNC2IP1+NO—0.32<em>MAC+0.42</em>MVK+0.74<em>HCHO+0.14</em>ISNI</td>
<td>k(T)=^B^/T \cdot A=1.4e-11,B=180</td>
</tr>
<tr>
<td>RO2IP1+NO2+R02IP1+0.78<em>HO2+0.86</em>NO2</td>
<td>k(T)=^B^/T \cdot A=1.4e-11,B=180</td>
</tr>
<tr>
<td>MVK02+NO—0.266<em>MGLYOX+0.266</em>HCHO+0.684<em>CH3CHO+0.684</em>CH3COO+0.15<em>ISNI+0.15</em>HCHO+0.15<em>H2O+0.15</em>HO2+0.15*NO2</td>
<td>k(T)=^B^/T \cdot A=1.4e-11,B=180</td>
</tr>
<tr>
<td>CH3COZ+NO—CH3COE+HO2+NO2</td>
<td>k(T)=^B^/T \cdot A=1.4e-11,B=180</td>
</tr>
<tr>
<td>APIOH+NO—0.8<em>CH3CHO+0.8</em>CH3COE+0.8<em>NO2+0.8</em>HO2+0.8<em>HO2+0.8</em>ISNI</td>
<td>k=4e-12</td>
</tr>
<tr>
<td>organic</td>
<td></td>
</tr>
<tr>
<td>CH3H2+NO—CH3OH</td>
<td>k(T)=^B^/T \cdot A=4.1e-13,B=790</td>
</tr>
<tr>
<td>C2H502+H2O—EETO2H</td>
<td>k(T)=^B^/T \cdot A=2.7e-13,B=1000</td>
</tr>
<tr>
<td>CH3COO+H2O—0.67<em>PPA+0.33</em>O3</td>
<td>k(T)=^B^/T \cdot A=4.3e-13,B=1040</td>
</tr>
<tr>
<td>SECC4H+HO2—BUO2H</td>
<td>k(T)=^B^/T \cdot A=2.7e-13,B=1000</td>
</tr>
<tr>
<td>CH3COX+H2O—CH4COX</td>
<td>k(T)=^B^/T \cdot A=2.7e-13,B=1000</td>
</tr>
<tr>
<td>CH2O2C+H2O—CH3O2C</td>
<td>k(T)=^B^/T \cdot A=2.7e-13,B=1000</td>
</tr>
<tr>
<td>C3H6+H2O—CH4CHX</td>
<td>k(T)=^B^/T \cdot A=2.7e-13,B=1000</td>
</tr>
<tr>
<td>OXYL1+HO2—OXYLH1</td>
<td>k(T)=^B^/T \cdot A=2.7e-13,B=1000</td>
</tr>
<tr>
<td>MEMAL1+H2O—MEMALH</td>
<td>k(T)=^B^/T \cdot A=2.7e-13,B=1000</td>
</tr>
<tr>
<td>Reactions</td>
<td>Kinetic constants</td>
</tr>
<tr>
<td>-----------------------------------------------</td>
<td>----------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>MEMAL2+HO2→MEMAH2</td>
<td>$k(T) = A e^{-B/T}$, A = 2.7 · 10^{-13}, B = 1000</td>
</tr>
<tr>
<td>RO2IP1+HO2→PEROX</td>
<td>$k(T) = A e^{-B/T}$, A = 2.7 · 10^{-13}, B = 1000</td>
</tr>
<tr>
<td>MACO2+HO2→MACO2H</td>
<td>$k(T) = A e^{-B/T}$, A = 2.7 · 10^{-13}, B = 1000</td>
</tr>
<tr>
<td>MVKO2+HO2→MVKO2H</td>
<td>$k(T) = A e^{-B/T}$, A = 2.7 · 10^{-13}, B = 1000</td>
</tr>
<tr>
<td>CH3COZ+HO2→CH4COZ</td>
<td>$k(T) = A e^{-B/T}$, A = 2.7 · 10^{-13}, B = 1000</td>
</tr>
<tr>
<td>APIOH+HO2→APIO2H</td>
<td>$k(T) = A e^{-B/T}$, A = 2.7 · 10^{-13}, B = 1000</td>
</tr>
<tr>
<td>CH3O2+CH3O2→2<em>HCHO+2</em>HO2</td>
<td>$k(T) = SPECIAL_1(1.1 · 10^{-13}, -365, 25, 1165)$</td>
</tr>
<tr>
<td>CH3O2+CH3O2→HCHO+CH3OH</td>
<td>$k(T) = SPECIAL_2(2.1 · 10^{-13}, -365, 25, 1165)$</td>
</tr>
<tr>
<td>C2H5O2+CH3O2→CH3CHO+HCHO+2*HO2</td>
<td>$k(T) = SPECIAL_3(3.6 · 10^{-14}, 0.1, 1.1 · 10^{-13}, -365, 10.2, 533, 25, 1165)$</td>
</tr>
<tr>
<td>C2H5O2+CH3O2→CH3CHO+CH3OH</td>
<td>$k(T) = SPECIAL_4(4.6 · 10^{-14}, 0.1, 1.1 · 10^{-13}, -365, 10.2, 533, 25, 1165)$</td>
</tr>
<tr>
<td>C2H5O2+CH3O2→CH2O2+CH3O2</td>
<td>$k(T) = SPECIAL_5(1.1 · 10^{-13}, -365, 25, 1165)$</td>
</tr>
<tr>
<td>C2H5O2+CH3O2→CH2O2+CH3O2</td>
<td>$k(T) = SPECIAL_6(1.1 · 10^{-13}, -365, 25, 1165)$</td>
</tr>
<tr>
<td>C2H5O2+CH3O2→CH2O2+CH3O2</td>
<td>$k(T) = SPECIAL_7(1.1 · 10^{-13}, -365, 25, 1165)$</td>
</tr>
<tr>
<td>C2H5O2+CH3O2→CH2O2+CH3O2</td>
<td>$k(T) = SPECIAL_8(1.1 · 10^{-13}, -365, 25, 1165)$</td>
</tr>
<tr>
<td>CH3CHX+CH3O2→CH3CHO+2<em>HCHO+2</em>HO2</td>
<td>$k(T) = SPECIAL_9(5.5 · 10^{-11}, 1.1 · 10^{-13}, -365, 10.2, 533, 25, 1165)$</td>
</tr>
<tr>
<td>CH3CHX+CH3O2→CH3CHO+2<em>HCHO+2</em>HO2</td>
<td>$k(T) = SPECIAL_10(5.5 · 10^{-11}, 1.1 · 10^{-13}, -365, 10.2, 533, 25, 1165)$</td>
</tr>
<tr>
<td>CH3CHX+CH3O2→CH3CHO+2<em>HCHO+2</em>HO2</td>
<td>$k(T) = SPECIAL_11(5.5 · 10^{-11}, 1.1 · 10^{-13}, -365, 10.2, 533, 25, 1165)$</td>
</tr>
<tr>
<td>CH3CHX+CH3O2→CH3CHO+2<em>HCHO+2</em>HO2</td>
<td>$k(T) = SPECIAL_12(5.5 · 10^{-11}, 1.1 · 10^{-13}, -365, 10.2, 533, 25, 1165)$</td>
</tr>
<tr>
<td>CH3CHX+CH3O2→CH3CHO+2<em>HCHO+2</em>HO2</td>
<td>$k(T) = SPECIAL_13(5.5 · 10^{-11}, 1.1 · 10^{-13}, -365, 10.2, 533, 25, 1165)$</td>
</tr>
<tr>
<td>CH3CHX+CH3O2→CH3CHO+2<em>HCHO+2</em>HO2</td>
<td>$k(T) = SPECIAL_14(5.5 · 10^{-11}, 1.1 · 10^{-13}, -365, 10.2, 533, 25, 1165)$</td>
</tr>
<tr>
<td>CH3CHX+CH3O2→CH3CHO+2<em>HCHO+2</em>HO2</td>
<td>$k(T) = SPECIAL_15(5.5 · 10^{-11}, 1.1 · 10^{-13}, -365, 10.2, 533, 25, 1165)$</td>
</tr>
</tbody>
</table>
Reactions | Kinetic constants
--- | ---
RO2IP1+CH3O2→0.3*MVK+0.3*MAC+1.6*HCHO+2*HO2 | k(T)=SPECIAL_3(1.3e-11,800,1.1e-13,-365,50,1165,25,1165)
RO2IP1+CH3O2→0.3*MVK+0.3*MAC+0.6*HCHO+CH3OH | k(T)=SPECIAL_4(1.3e-11,800,1.1e-13,-365,50,1165,25,1165)
RO2IP1+CH3O2→0.3*MVK+0.3*MAC+1.6*HCHO | k(T)=SPECIAL_4(1.3e-11,800,1.1e-13,-365,50,1165,25,1165)
RNC5H8+CH3O2→0.6*ISNI+HCHO+2*HO2 | k(T)=SPECIAL_3(1.3e-11,800,1.1e-13,-365,50,1165,25,1165)
RNC5H8+CH3O2→0.6*ISNI+CH3OH | k(T)=SPECIAL_4(1.3e-11,800,1.1e-13,-365,50,1165,25,1165)
RNC5H8+CH3O2→0.6*ISNI+HCHO | k(T)=SPECIAL_4(1.3e-11,800,1.1e-13,-365,25,1165,50,1165)
MACO2+CH3O2→CH3COZ+CO2+HCHO+HO2 | k(T)=SPECIAL_1(5.1e-12,-272,4.4e5,3910)
MACO2+CH3O2→MAA+HCHO | k(T)=SPECIAL_2(5.1e-12,-272,4.4e5,3910)
MVKO2+CH3O2→MGLYOX+2*HCHO+2*HO2 | k(T)=SPECIAL_3(5.5e-11,1500,1.1e-13,-365,50,1165,25,1165)
MVKO2+CH3O2→MGLYOX+CH3OH | k(T)=SPECIAL_4(5.5e-11,1500,1.1e-13,-365,50,1165,25,1165)
MVKO2+CH3O2→MGLYOX+HCHO+CH3OH | k(T)=SPECIAL_4(5.5e-11,1500,1.1e-13,-365,50,1165,25,1165)
APIOH+CH3O2→CH3CHO+CH3COE+HCHO+2*HO2 | k(T)=SPECIAL_3(1.8e-11,2200,1.1e-13,-365,1e9,0,25,1165)
APIOH+CH3O2→CH3CHO+CH3COE+HCHO | k(T)=SPECIAL_4(1.8e-11,2200,1.1e-13,-365,1e9,0,25,1165)
APINO3+CH3O2→CH3CHO+CH3COE+NO2+HCHO+HO2 | k(T)=SPECIAL_3(1.8e-11,2200,1.1e-13,-365,1e9,0,25,1165)
APINO3+CH3O2→ORNIT2+HCHO | k(T)=SPECIAL_4(1.8e-11,2200,1.1e-13,-365,1e9,0,25,1165)
CH3COO+CH3COO→2.*CH3O2+2.*CO2 | k(T)=Ae^{-B/T},A=2.8e-12,B=-530
C2H5O2+CH3COO→CH3CHO+CH3O2+CO2+HO2 | k(T)=SPECIAL_3(6.4e-14,0,2.8e-12,-530,10.2,533,1e9,0)
C2H5O2+CH3COO→CH3CHO+MECOOH | k(T)=SPECIAL_4(6.4e-14,0,2.8e-12,-530,1e9,0,10.2,533)
SECC4H+CH3COO→SECBUO+CH3O2+CO2 | k(T)=SPECIAL_3(1.2e-12,1500,2.8e-12,-530,1e9,0,50,1165)
SECC4H+CH3COO→CH3COE+MECOOH | k(T)=SPECIAL_4(1.2e-12,1500,2.8e-12,-530,1e9,0,50,1165)
CH3CHX+CH3COO→CH3CHO+HCHO+CH3O2+CO2+HO2 | k(T)=SPECIAL_3(1.2e-10,2200,2.8e-12,-365,50,1165,25,1165)
CH3CHX+CH3COO→CH3CHO+HCHO+MECOOH | k(T)=SPECIAL_4(1.2e-10,2200,2.8e-12,-365,50,1165,25,1165)
RNC3H6+CH3COO→0.5*CARNIT+0.5*HCHO+0.5*CH3CHO+0.5*NO2+CH3O2+CO2+0.5*HO2 | k(T)=SPECIAL_3(1.2e-10,2200,2.8e-12,-365,50,1165,25,1165)
RNC3H6+CH3COO→ORNIT1+MECOOH | k(T)=SPECIAL_4(1.2e-10,2200,2.8e-12,-365,50,1165,25,1165)
<table>
<thead>
<tr>
<th>Reactions</th>
<th>Kinetic constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>R0H2IP+CH3COO→0.3<em>MVK+0.3</em>MAC+0.6*HCHO+MECOOH</td>
<td>k(T)=SPECIAL_4(1.3e-11,800,2.8e-12,-530,1e9,0,50,1165)</td>
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<tr>
<td>RNC5H8+CH3COO→0.6*ISNI+CH3O2+CO2</td>
<td>k(T)=SPECIAL_3(1.3e-11,800,2.8e-12,-530,1e9,0,50,1165)</td>
</tr>
<tr>
<td>RNC5H8+CH3COO→0.6*ISNI+MECOOH</td>
<td>k(T)=SPECIAL_4(1.3e-11,800,2.8e-12,-530,1e9,0,50,1165)</td>
</tr>
<tr>
<td>MACO2+CH3COO→CH3O2+CH3COE+2*CO2</td>
<td>k(T)=Ac^{-B/T}, A=5.6e-12, B=530</td>
</tr>
<tr>
<td>MVKO2+CH3COO→MGLYOX+HCHO+HO2+CH3O2+CO2</td>
<td>k(T)=SPECIAL_3(5.5e-11,1500,2.8e-12,-530,1e9,0,50,1165)</td>
</tr>
<tr>
<td>MVKO2+CH3COO→MGLYOX+HCHO+MECOOH</td>
<td>k(T)=SPECIAL_4(5.5e-11,1500,2.8e-12,-530,1e9,0,50,1165)</td>
</tr>
<tr>
<td>APIOH+CH3COO→CH3CHO+CH3COE+HO2+CH3O2+CO2</td>
<td>k(T)=Ac^{-B/T}, A=1.8e-11, B=2200</td>
</tr>
<tr>
<td>APINO3+CH3COO→CH3CHO+CH3COE+NO2+CH3O2+CO2</td>
<td>k(T)=Ac^{-B/T}, A=1.4e-11, B=835</td>
</tr>
<tr>
<td>C2H5O2+C2H5O2→2<em>CH3CHO+2</em>HO2</td>
<td>k(T)=SPECIAL_1(6.4e-14,0,10.2,533)</td>
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<tr>
<td>C2H5O2+C2H5O2→CH3CHO+C2H5OH</td>
<td>k(T)=SPECIAL_2(6.4e-14,0,10.2,533)</td>
</tr>
<tr>
<td>SECC4H+SECC4H→2*SECBUO</td>
<td>k(T)=SPECIAL_1(1.2e-12,1500,50,1165)</td>
</tr>
<tr>
<td>SECC4H+SECC4H→2*CH3COE</td>
<td>k(T)=SPECIAL_2(1.2e-12,1500,50,1165)</td>
</tr>
<tr>
<td>CH2O2C+CH2O2C→4<em>HCHO+2</em>HO2</td>
<td>k(T)=SPECIAL_1(2.3e-12,0,50,1165)</td>
</tr>
<tr>
<td>CH2O2C+CH2O2C→4*HCHO</td>
<td>k(T)=SPECIAL_2(2.3e-12,0,50,1165)</td>
</tr>
<tr>
<td>CH3CHX+CH3CHX→2<em>HCHO+2</em>CH3CHO+2*HO2</td>
<td>k(T)=SPECIAL_1(1.3e-10,2200,50,1165)</td>
</tr>
<tr>
<td>CH3CHX+CH3CHX→2<em>HCHO+2</em>CH3CHO</td>
<td>k(T)=SPECIAL_2(1.3e-10,2200,50,1165)</td>
</tr>
<tr>
<td>RNC3H6+RNC3H6→CARNIT+HO2+HCHO+CH3CHO+NO2</td>
<td>k(T)=SPECIAL_1(1.3e-10,2200,50,1165)</td>
</tr>
<tr>
<td>ORGCH3X+ORGCH3X→2<em>HCHO+2</em>CH3CHO</td>
<td>k(T)=SPECIAL_2(1.3e-10,2200,50,1165)</td>
</tr>
<tr>
<td>MEMAL1+MEMAL1→2<em>GLYOX+2</em>MGLYOX+2*HO2</td>
<td>k(T)=SPECIAL_1(1.3e-11,800,50,1165)</td>
</tr>
<tr>
<td>MEMAL1+MEMAL1→2<em>GLYOX+2</em>MGLYOX</td>
<td>k(T)=SPECIAL_2(1.3e-11,800,50,1165)</td>
</tr>
<tr>
<td>MEMAL2+MEMAL2→2<em>MALEIC+2</em>CH3O2</td>
<td>k(T)=Ac^{-B/T}, A=2.8e-12, B=530</td>
</tr>
<tr>
<td>RO2IP1+RO2IP1→0.6<em>MVK+0.6</em>MAC+1.2<em>HCHO+1.2</em>HO2</td>
<td>k(T)=Ac^{-B/T}, A=1.4e-11, B=835</td>
</tr>
<tr>
<td>RO2IP1+RO2IP1→0.6<em>MVK+0.6</em>MAC+1.2*HCHO</td>
<td>k(T)=Ac^{-B/T}, A=1.4e-11, B=835</td>
</tr>
<tr>
<td>RNC5H8+RNC5H8→1.2<em>ISNI+1.2</em>HO2</td>
<td>k(T)=Ac^{-B/T}, A=1.4e-11, B=835</td>
</tr>
<tr>
<td>RNC5H8+RNC5H8→1.2*ISNI</td>
<td>k(T)=Ac^{-B/T}, A=1.4e-11, B=835</td>
</tr>
<tr>
<td>MACO2+MACO2→2<em>CH3CO2+2</em>CO2</td>
<td>k(T)=Ac^{-B/T}, A=2.8e-12, B=530</td>
</tr>
<tr>
<td>MVKO2+MVKO2→2<em>MGLYOX+2</em>HCHO+2*HO2</td>
<td>k(T)=SPECIAL_1(1.3e-11,800,50,1165)</td>
</tr>
<tr>
<td>MVKO2+MVKO2→2<em>MGLYOX+2</em>HCHO</td>
<td>k(T)=SPECIAL_2(1.3e-11,800,50,1165)</td>
</tr>
<tr>
<td>R02IP1+R02IP1→0.6<em>MVK+0.6</em>MAC+1.2*HCHO</td>
<td>k(T)=SPECIAL_1(1.3e-11,800,50,1165)</td>
</tr>
<tr>
<td>ROXYL1+NO→BENZAL+NO2+HO2</td>
<td>k(T)=Ac^{-B/T}, A=2.8e-12, B=530</td>
</tr>
<tr>
<td>CH3NO3+OH→HCHO+HNO3+H2O</td>
<td>k(T)=Ac^{-B/T}, A=2.8e-12, B=530</td>
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<td>CH3NO3+OH→HCHO+HNO3+H2O</td>
<td>k(T)=Ac^{-B/T}, A=2.8e-12, B=530</td>
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<td>ROXYL1+NO→BENZAL+NO2+HO2</td>
<td>k(T)=Ac^{-B/T}, A=2.8e-12, B=530</td>
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<td>RNC3H6+RNC3H6→CARNIT+HO2+HCHO+CH3CHO+NO2</td>
<td>k(T)=Ac^{-B/T}, A=2.8e-12, B=530</td>
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<tr>
<td>RNC3H6+RNC3H6→CARNIT+HO2+HCHO+CH3CHO+NO2</td>
<td>k(T)=Ac^{-B/T}, A=2.8e-12, B=530</td>
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<td>ROXYL1+NO→BENZAL+NO2+HO2</td>
<td>k(T)=Ac^{-B/T}, A=2.8e-12, B=530</td>
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<td>CH3NO3+OH→HCHO+HNO3+H2O</td>
<td>k(T)=Ac^{-B/T}, A=2.8e-12, B=530</td>
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<td>ROXYL1+NO→BENZAL+NO2+HO2</td>
<td>k(T)=Ac^{-B/T}, A=2.8e-12, B=530</td>
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<td>CH3NO3+OH→HCHO+HNO3+H2O</td>
<td>k(T)=Ac^{-B/T}, A=2.8e-12, B=530</td>
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</table>
Reactions Kinetic constants

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<tbody>
<tr>
<td>RNC2H4+HO2→ORNIT1</td>
<td>$k(T) = Ae^{-B/T}, A=2.7\times10^{-13}, B=-1000$</td>
</tr>
<tr>
<td>RNC3H6+HO2→ORNIT1</td>
<td>$k(T) = Ae^{-B/T}, A=2.7\times10^{-13}, B=-1000$</td>
</tr>
<tr>
<td>ROXYL1+HO2→BENZYL</td>
<td>$k(T) = Ae^{-B/T}, A=2.7\times10^{-13}, B=-1000$</td>
</tr>
<tr>
<td>ISNIR+HO2→ORNIT2</td>
<td>$k(T) = Ae^{-B/T}, A=2.7\times10^{-13}, B=-1000$</td>
</tr>
<tr>
<td>APINO3+HO2→ORNIT2</td>
<td>$k(T) = Ae^{-B/T}, A=2.7\times10^{-13}, B=-1000$</td>
</tr>
<tr>
<td>CH3COO+NO2+M→PAN</td>
<td>$k(T,M) = troe(2.7\times10^{-28}, 0, 5.4\times10^{-16}, 1.2\times10^{-11}, 0, 0.9, 0.3)$</td>
</tr>
<tr>
<td>PAN+M→CH3COO+NO2</td>
<td>$k(T,M) = troe(4.9\times10^{-3}, 12100, 0, 5.4\times10^{16}, 13830, 0, 0.3)$</td>
</tr>
<tr>
<td>PAN+OH→HCHO+NO3+CO2</td>
<td>$k(T) = Ae^{-B/T}, A=9.5\times10^{-13}, B=650$</td>
</tr>
<tr>
<td>MACO2+NO2+M→MACPAN</td>
<td>$k(T,M) = troe(2.7\times10^{-28}, 0, 5.4\times10^{-16}, 1.2\times10^{-11}, 0, 0.9, 0.3)$</td>
</tr>
<tr>
<td>MACPAN+M→MACO2+NO2</td>
<td>$k(T,M) = troe(4.9\times10^{-3}, 12100, 0, 5.4\times10^{16}, 13830, 0, 0.3)$</td>
</tr>
<tr>
<td>MACPAN+OH→CH3COE+NO3+O3+CO2</td>
<td>$k(T) = Ae^{-B/T}, A=3.25\times10^{-13}, B=-500$</td>
</tr>
<tr>
<td>MEMAL2+NO2+M→MEMPAN</td>
<td>$k(T,M) = troe(2.7\times10^{-28}, 0, 5.4\times10^{-16}, 1.2\times10^{-11}, 0, 0.9, 0.3)$</td>
</tr>
<tr>
<td>MEMPAN+M→MEMAL2+NO2</td>
<td>$k(T,M) = troe(4.9\times10^{-3}, 12100, 0, 5.4\times10^{16}, 13830, 0, 0.3)$</td>
</tr>
<tr>
<td>MEMPAN+OH→CH3COE+NO3+O3+CO2</td>
<td>$k(T) = Ae^{-B/T}, A=3.25\times10^{-13}, B=650$</td>
</tr>
<tr>
<td>CH3O2+NO2+M→CH3NO4</td>
<td>$k(T) = troe(2.5\times10^{-30}, 0, 5.5, 7.5\times10^{-12}, 0, 0, 0.36)$</td>
</tr>
<tr>
<td>CH3NO4+M→CH3O2+NO2</td>
<td>$k(T) = troe(9\times10^{-5}, 9690, 0, 1.1\times10^{16}, 10560, 0, 0.36)$</td>
</tr>
<tr>
<td>ORNIT1+OH→CARNIT+OH</td>
<td>$k(T) = Ae^{-B/T}(300/T)^{\frac{N}{3}}, A=6.1\times10^{-14}, B=-1743, N=-2$</td>
</tr>
<tr>
<td>ORNIT1+OH→RNC3H6</td>
<td>$k(T) = Ae^{-B/T}, A=1.9\times10^{-12}, B=-190$</td>
</tr>
<tr>
<td>ORNIT2+OH→0.95<em>CH3CHO+0.475</em>CH3COE+0.475<em>MGLYOX+0.05</em>ISNI+0.05<em>OH+0.95</em>NO2</td>
<td>$k(T) = Ae^{-B/T}(300/T)^{\frac{N}{3}}, A=6.1\times10^{-14}, B=-1743, N=-2$</td>
</tr>
<tr>
<td>ORNIT2+OH→ISNIR</td>
<td>$k(T) = Ae^{-B/T}, A=1.9\times10^{-12}, B=-190$</td>
</tr>
</tbody>
</table>

**Photolytic**

<table>
<thead>
<tr>
<th>Reaction</th>
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</tr>
</thead>
<tbody>
<tr>
<td>O3→2*OH</td>
<td>$J(T,Z,H2O) = photorate(O3)$</td>
</tr>
<tr>
<td>NO2→NO+O3</td>
<td>$J(Z) = photorate(NO2)$</td>
</tr>
<tr>
<td>NO3→NO2+O3</td>
<td>$J(Z) = photorate(NO3-2)$</td>
</tr>
<tr>
<td>H2O2→2*OH</td>
<td>$J(Z) = photorate(H2O2)$</td>
</tr>
<tr>
<td>HNO3→NO2+OH</td>
<td>$J(Z) = photorate(HNO3)$</td>
</tr>
<tr>
<td>HCHO→CO+2*HO2</td>
<td>$J(Z) = photorate(HCHO)$</td>
</tr>
<tr>
<td>HCHO→CO+H2</td>
<td>$J(Z) = photorate(HCHO-2)$</td>
</tr>
<tr>
<td>CH3CHO→CH3O2+HO2+CO</td>
<td>$J(Z) = photorate(CH3CHO)$</td>
</tr>
<tr>
<td>CH3COE→CH3COO+2H5O2</td>
<td>$J(Z) = photorate(CH3COE)$</td>
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<tr>
<td>CH3COY→2*CH3COO</td>
<td>$J(Z) = photorate(CH3COY)$</td>
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<tr>
<td>MGLYOX→CH3COO+HO2+CO</td>
<td>$J(Z) = photorate(MGLYOX)$</td>
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<tr>
<td>GLYOX→0.6<em>HO2+2</em>CO+1.4*H2</td>
<td>$J(Z) = photorate(GLYOX)$</td>
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<tr>
<td>MEMALD→0.5<em>OFURAN+0.5</em>MEMAL2+0.5*HO2</td>
<td>$J(Z) = photorate(MEMALD)$</td>
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<tr>
<td>NO3→NO</td>
<td>$J(Z) = photorate(NO3-1)$</td>
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<tr>
<td>NO2→NO2+NO3</td>
<td>$J(Z) = photorate(NO2)$</td>
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<tr>
<td>CH3O2H→HCHO+OH+HO2</td>
<td>$J(Z) = photorate(CH3O2H)$</td>
</tr>
<tr>
<td>ETO2H→CH3CHO+OH+HO2</td>
<td>$J(Z) = photorate(CH3O2H)$</td>
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<tr>
<td>BUO2H→CH3COE+OH+HO2</td>
<td>$J(Z) = photorate(CH3O2H)$</td>
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<tr>
<td>CH4OX→CH3COY+OH+HO2</td>
<td>$J(Z) = photorate(CH3O2H)$</td>
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<tr>
<td>CH3O2C→2*HCHO+OH+HO2</td>
<td>$J(Z) = photorate(CH3O2H)$</td>
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<tr>
<td>CH4CHX→HCHO+CH3CHO+OH+HO2</td>
<td>$J(Z) = photorate(CH3O2H)$</td>
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<tr>
<td>OXYLH1→MEMALD+MGLYOX+OH+HO2</td>
<td>$J(Z) = photorate(CH3O2H)$</td>
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<tr>
<td>MEMALH→GLYOX+MGLYOX+OH+HO2</td>
<td>$J(Z) = photorate(CH3O2H)$</td>
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<tr>
<td>MEMAH2→MALEIC+OH+CH3O2</td>
<td>$J(Z) = photorate(CH3O2H)$</td>
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<tr>
<td>PEROX→0.14<em>R02IP1+0.488</em>CH3COE+0.372<em>MAC+0.86</em>HCHO+0.9*HO2+OH</td>
<td>$J(Z) = photorate(CH3O2H)$</td>
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<tr>
<td>MACO2H→CH3COZ+OH+CO2</td>
<td>$J(Z) = photorate(CH3O2H)$</td>
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<tr>
<td>MVKO2H→0.28<em>HCHO+0.28</em>MGLYOX+0.28<em>HO2+0.72</em>CH3CHO+0.72*CH3COO+OH</td>
<td>$J(Z) = photorate(CH3O2H)$</td>
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<tr>
<td>CH4COZ→CH3COE+OH+HO2</td>
<td>$J(Z) = photorate(CH3O2H)$</td>
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<tr>
<td>APIO2H→CH3CHO+CH3COE+OH+HO2</td>
<td>$J(Z) = photorate(CH3O2H)$</td>
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<tr>
<td>PPA→CH3O2+CO2+OH</td>
<td>$J(Z) = photorate(PPA)$</td>
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<tr>
<td>HNO4→HO2+NO2</td>
<td>$J(Z) = photorate(HNO4)$</td>
</tr>
<tr>
<td>HONO→NO+OH</td>
<td>$J(Z) = photorate(HONO)$</td>
</tr>
<tr>
<td>CH3NO4→CH3O2+NO2</td>
<td>$J(Z) = photorate(CH3O2H)$</td>
</tr>
<tr>
<td>CH3NO3→HCHO+HO2+NO2</td>
<td>$J(Z) = photorate(CH3O2H)$</td>
</tr>
<tr>
<td>ETNO3→CH3CHO+HO2+NO2</td>
<td>$J(Z) = photorate(CH3O2H)$</td>
</tr>
</tbody>
</table>
### Kinetic constants

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Kinetic constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>BunO3→CH3CO+H2O+NO2</td>
<td>J(Z)=photorate(BunO3)</td>
</tr>
<tr>
<td>Pan→CH3CO+NO2</td>
<td>J(Z)=photorate(Pan)</td>
</tr>
<tr>
<td>CarNit→CH3CHO+CH3CO+NO2</td>
<td>J(Z)=photorate(CH3CHO)</td>
</tr>
<tr>
<td>OrNit1→CH3CHO+HCHO+NO2+OH</td>
<td>J(Z)=photorate(CH3O2H)</td>
</tr>
<tr>
<td>OrNit2→0.95<em>CH3CHO+0.475</em>CH3COE+0.475<em>Mglyox+0.05</em>isni+0.05<em>H2O+0.95</em>NO2+OH</td>
<td>J(Z)=photorate(CH3O2H)</td>
</tr>
<tr>
<td>ApiNe+NO3→Apino3</td>
<td>k(T)=A0e(^{-B0/T}), A=1.19e-12, B=-490</td>
</tr>
<tr>
<td>BpRNe+NO3→Apino3</td>
<td>k(T)=A0e(^{-B0/T}), A=1.19e-12, B=-490</td>
</tr>
<tr>
<td>LimO+NO3→Apino3</td>
<td>k(T)=A0e(^{-B0/T}), A=1.19e-12, B=-490</td>
</tr>
<tr>
<td>OcimEn+NO3→Apino3</td>
<td>k(T)=A0e(^{-B0/T}), A=1.19e-12, B=-490</td>
</tr>
<tr>
<td>TerpEn+NO3→Apino3</td>
<td>k(T)=A0e(^{-B0/T}), A=1.19e-12, B=-490</td>
</tr>
<tr>
<td>HumulEn+NO3→Apino3</td>
<td>k(T)=A0e(^{-B0/T}), A=1.19e-12, B=-490</td>
</tr>
<tr>
<td>ApiNe+OH→ApiOH</td>
<td>k(T)=A0e(^{-B0/T}), A=1.21e-11, B=-444</td>
</tr>
<tr>
<td>BpRNe+OH→ApiOH</td>
<td>k(T)=A0e(^{-B0/T}), A=1.21e-11, B=-444</td>
</tr>
<tr>
<td>LimO+OH→ApiOH</td>
<td>k(T)=A0e(^{-B0/T}), A=1.21e-11, B=-444</td>
</tr>
<tr>
<td>OcimEn+OH→ApiOH</td>
<td>k(T)=A0e(^{-B0/T}), A=1.21e-11, B=-444</td>
</tr>
<tr>
<td>TerpEn+OH→ApiOH</td>
<td>k(T)=A0e(^{-B0/T}), A=1.21e-11, B=-444</td>
</tr>
<tr>
<td>HumulEn+OH→ApiOH</td>
<td>k(T)=A0e(^{-B0/T}), A=1.21e-11, B=-444</td>
</tr>
<tr>
<td>ApiNe+O3→0.65<em>CH3CHO+0.53</em>CH3COE+0.14<em>CO+0.2</em>C2H5O2+0.42<em>CH3CHX+0.85</em>OH+0.1*HO2</td>
<td>k(T)=A0e(^{-B0/T}), A=1.0e-15, B=736</td>
</tr>
<tr>
<td>BpRNe+O3→0.65<em>CH3CHO+0.53</em>CH3COE+0.14<em>CO+0.2</em>C2H5O2+0.42<em>CH3CHX+0.85</em>OH+0.1*HO2</td>
<td>k(T)=A0e(^{-B0/T}), A=1.0e-15, B=736</td>
</tr>
<tr>
<td>LimO+O3→0.65<em>CH3CHO+0.53</em>CH3COE+0.14<em>CO+0.2</em>C2H5O2+0.42<em>CH3CHX+0.85</em>OH+0.1*HO2</td>
<td>k(T)=A0e(^{-B0/T}), A=1.0e-15, B=736</td>
</tr>
<tr>
<td>OcimEn+O3→0.65<em>CH3CHO+0.53</em>CH3COE+0.14<em>CO+0.2</em>C2H5O2+0.42<em>CH3CHX+0.85</em>OH+0.1*HO2</td>
<td>k(T)=A0e(^{-B0/T}), A=1.0e-15, B=736</td>
</tr>
<tr>
<td>TerpEn+O3→0.65<em>CH3CHO+0.53</em>CH3COE+0.14<em>CO+0.2</em>C2H5O2+0.42<em>CH3CHX+0.85</em>OH+0.1*HO2</td>
<td>k(T)=A0e(^{-B0/T}), A=1.0e-15, B=736</td>
</tr>
<tr>
<td>HumulEn+O3→0.65<em>CH3CHO+0.53</em>CH3COE+0.14<em>CO+0.2</em>C2H5O2+0.42<em>CH3CHX+0.85</em>OH+0.1*HO2</td>
<td>k(T)=A0e(^{-B0/T}), A=1.0e-15, B=736</td>
</tr>
<tr>
<td>C5H8+OH→RO2ip1</td>
<td>k(T)=A0e(^{-B0/T}), A=2.55e-11, B=-410</td>
</tr>
<tr>
<td>NC4H10+OH→secc4H</td>
<td>k(T)=A0e(^{-B0/(300/T)2}), A=1.36e-12, B=-190, N=-2</td>
</tr>
<tr>
<td>OxyL+OH→OxyL1</td>
<td>k=1.37e-11</td>
</tr>
</tbody>
</table>

- The reactions O3+hν→O(1D), O(1D)+H2O→2OH, O(1D)+M→O(3P)+M and O(3P)+O2+M→O3+M have been combined to reaction O3+hν→O(1D) by taking into account H2O and M concentrations in order to adjust the photolysis frequency.
- Due to lack of data, photolysis frequencies of higher organic peroxides are taken as that of CH3OOH.
- Three body Troe reactions [1], given in the form:

  \[ k = \frac{k_0[M]}{1 + \frac{k_0[M]}{k_∞} f Z} \]

  with

  \[ Z = \frac{1}{1 + \left( \log_{10} \left( \frac{k_0(T)[M]}{k_∞(T)} \right) \right)^2} \]

  \[ k_0 = A_0 e \left( -\frac{B_0}{T} \right) \left( \frac{T}{300} \right)^{-n}, \text{ and } k_∞ = A_∞ e \left( -\frac{B_∞}{T} \right) \left( \frac{T}{300} \right)^{-m}, \]

  The parameters are given in the order \( A_0, B_0, n, A_∞, B_∞, m, f \).

- The reaction NO2+OH:

  \[ k = \frac{k_0[M]}{1 + \frac{k_0[M]}{k_∞} f Z} \]
The parameters are given in the order $A_0, B_0, n, A_\infty, B_\infty, m, f$

- Radical recombinations SPECIAL_1:
  \[ k(T) = k_1(T) \times \frac{k_2(T)}{1 + k_2(T)} \]

  The parameters are given in the order $A_1, B_1, A_2, B_2$

- Radical recombinations SPECIAL_2:
  \[ k(T) = \frac{k_1(T)}{1 + k_2(T)} \]

  The parameters are given in the order $A_1, B_1, A_2, B_2$

- Radical recombinations SPECIAL_3:
  \[ k(T) = 2 \times \sqrt{k_1(T) \times k_2(T) \times k_3(T) \times k_4(T)} \]

  The parameters are given in the order $A_1, B_1, A_2, B_2, A_3, B_3, A_4, B_4$

- Radical recombinations SPECIAL_4:
  \[ k(T) = 2 \times \sqrt{k_1(T) \times k_2(T)} \times \frac{1 - \sqrt{k_3(T) \times k_4(T) \times (1 - k_3(T) \times k_4(T))}}{2 - \frac{k_3(T)}{1 + k_3(T)} - \frac{k_4(T)}{1 + k_4(T)}} \]

  The parameters are given in the order $A_1, B_1, A_2, B_2, A_3, B_3, A_4, B_4$

10.2.3 Species list of the reduced MELCHIOR2 gas-phase chemical mechanism

<table>
<thead>
<tr>
<th>Species</th>
<th>Definition</th>
<th>Hydrocarbon species</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inorganic compounds</td>
<td></td>
<td>H2SO4</td>
</tr>
<tr>
<td>O3</td>
<td>ozone</td>
<td>CH4</td>
</tr>
<tr>
<td>H2O2</td>
<td>hydrogen peroxide</td>
<td>C2H6</td>
</tr>
<tr>
<td>OH</td>
<td>hydroxyl radical</td>
<td>NC4H10</td>
</tr>
<tr>
<td>HO2</td>
<td>hydroperoxy radical</td>
<td>C2H4</td>
</tr>
<tr>
<td>NO</td>
<td>nitric oxide</td>
<td>C3H6</td>
</tr>
<tr>
<td>NO2</td>
<td>nitrogen dioxide</td>
<td>OXYL</td>
</tr>
<tr>
<td>NO3</td>
<td>nitrogen trioxide</td>
<td>C5H8</td>
</tr>
<tr>
<td>N2O5</td>
<td>dinitrogen pentoxide</td>
<td>APINEN</td>
</tr>
<tr>
<td>HONO</td>
<td>nitrous acid</td>
<td>BPINEN</td>
</tr>
<tr>
<td>HNO3</td>
<td></td>
<td>LIMONE</td>
</tr>
<tr>
<td>CO</td>
<td>carbon monoxide</td>
<td>TERPEN</td>
</tr>
<tr>
<td>SO2</td>
<td>sulfur dioxide</td>
<td>HUMULE</td>
</tr>
<tr>
<td></td>
<td></td>
<td>OCIMEN</td>
</tr>
</tbody>
</table>

\(^{1}\)Hydrocarbon model species (except for CH4 and C2H4) represent groups of hydrocarbons with similar reactivity. As “definition” a typical representative of this group is given. This is also true for the degradation products.
Carbonyls
HCHO ................................. formaldehyde
CH3CHO ............................. acetaldehyde
CH3COE .............................. methyl ethyl ketone
GLYOX .............................. glyoxal
MGLYOX ............................. methyl glyoxal
CH3COY .............................. dimethyl glyoxal
MEMALD ............................. unsaturated dicarbonyls, reacting like 4-oxo-2-pentenal
MVK ................................. methyl vinyl ketone
MAC ................................. methacroleine

Organic nitrates
PAN ................................. peroxyacetyl nitrate
CARNIT .............................. nitrate carbonyl taken as α-nitrooxy acetone
ISNI ................................. unsaturated nitrate from isoprene degradation

Organic peroxides
CH3O2H .............................. methyl hydroperoxide
PPA ................................. peroxy acetyl acid

(Per)oxy radicals
CH3O2 ............................... methyl peroxy radical
CH3COO .............................. peroxy acetyl radical

Operators 3
oRO2 ............................... representing peroxy radicals from OH attack to C2H5, NCHH10, C2H4, C3H6, OXYL, CH3COE, MEMALD, and MVK
oROOH ............................. representing organic peroxides from oRO2+HO2 reactions
obio ............................... representing peroxy radicals produced by C5H8 and APINEN + OH reaction
obioH ............................... representing biogenic organic peroxides from obio+HO2 and obio+obio reactions
oPAN ............................... representing PAN homologue compounds (except PAN)
PANH ............................... representing results from oPAN+HO2 reaction
toPAN ............................... representing results from oPAN+NO2 reaction
oRN1 ............................... representing organic nitrate peroxy radicals from NO3 attack to C2H4, C3H6, C5H8, APINEN, BPINEN, LIMONE, TERPEN, OCIMEN, HUMULE and OH attack to ISNI

Reaction list of the reduced MELCHIOR2 chemical mechanism

<table>
<thead>
<tr>
<th>Reactions</th>
<th>Kinetic constants</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>O3+NO→NO2</td>
<td>Ac<strong>B/T</strong>,A=1.8e-12,B=1370</td>
<td>[1]</td>
</tr>
<tr>
<td>O3+NO2→NO3</td>
<td>Ac<strong>B/T</strong>,A=1.2e-13,B=2450</td>
<td>[1]</td>
</tr>
<tr>
<td>O3+OH→HO2</td>
<td>Ac<strong>B/T</strong>,A=1.9e-12,B=1000</td>
<td>[1]</td>
</tr>
<tr>
<td>O3+HO2→OH</td>
<td>Ac<strong>B/T</strong>,A=1.4e-14,B=600</td>
<td>[1]</td>
</tr>
<tr>
<td>NO+HO2→OH+NO2</td>
<td>Ac<strong>B/T</strong>,A=3.7e-12,B=240</td>
<td>[1]</td>
</tr>
<tr>
<td>NO2+OH+M→HNO3</td>
<td>troe(3.4e-30,3.2,4.77e-11,1.4,0.30)</td>
<td>[2], n9</td>
</tr>
<tr>
<td>H2O2+OH→H2O</td>
<td>Ac<strong>B/T</strong>,A=4.8e-11,B=250</td>
<td>[1]</td>
</tr>
<tr>
<td>H2O2+OH→HO2</td>
<td>Ac<strong>B/T</strong>,A=2.9e-12,B=160</td>
<td>[1]</td>
</tr>
<tr>
<td>HNO3+OH→NO3</td>
<td>Ac<strong>B/T</strong>,A=5.5e-15,B=985</td>
<td>[1], n1</td>
</tr>
<tr>
<td>CO+OH→HO2+CO2</td>
<td>Ac<strong>B/T</strong>(300/T)N, A=2e-13, B=0, N=1</td>
<td>[3], n1</td>
</tr>
<tr>
<td>H2O2+HO2→H2O2</td>
<td>Ac<strong>B/T</strong>,A=2.2e-13,B=740</td>
<td>[1], n1</td>
</tr>
<tr>
<td>H2O2+H2O→H2O2</td>
<td>Ac<strong>B/T</strong>,A=4.52e-34,B=2827</td>
<td>[1], n1</td>
</tr>
<tr>
<td>NO3→NO+HO2</td>
<td>4e-12</td>
<td>[1]</td>
</tr>
<tr>
<td>NO2+HNO3→HNO2+NO</td>
<td>2e-15</td>
<td>[3]</td>
</tr>
<tr>
<td>NO3+NO→2*NO2</td>
<td>Ac<strong>B/T</strong>,A=1.8e-11,B=110</td>
<td>[1]</td>
</tr>
<tr>
<td>NO2+NO→2*NO2</td>
<td>Ac<strong>B/T</strong>,A=4.5e-14,B=1260</td>
<td>[3]</td>
</tr>
<tr>
<td>NO2+NO→N2O5</td>
<td>troe(2e-30,0.3,4,2e-12,0.2,0.33)</td>
<td>[1], n9</td>
</tr>
<tr>
<td>N2O5→NO3+NO2</td>
<td>troe(1e-3,11000,3.5,9.7e14,11080,-0.1,0.33)</td>
<td>[1], n9</td>
</tr>
<tr>
<td>N2O5+H2O→2*HNO3</td>
<td>2.6e-22</td>
<td>[4]</td>
</tr>
<tr>
<td>NO+OH+M→HONO</td>
<td>troe(7e-31,0.2,6.1e-11,0.0,5.0,0.6)</td>
<td>[1], n9</td>
</tr>
<tr>
<td>HONO+OH→NO2</td>
<td>Ac<strong>B/T</strong>,A=1.8e-11,B=390</td>
<td>[1]</td>
</tr>
<tr>
<td>NO+NO+O2→2*NO2</td>
<td>Ac<strong>B/T</strong>,A=3.30E-39,B=530.0</td>
<td>[1]</td>
</tr>
<tr>
<td>NO+HONO→HONO</td>
<td>0.5*depo(NO2)</td>
<td>[18]</td>
</tr>
</tbody>
</table>

SOx chemistry

3For the concept of “chemical operators” see Carter (1990) and Aumont et al. (1997)
### OH attack to hydrocarbons

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Kinetic constants</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH4+OH→CH3O</td>
<td>$Ae^{-\frac{B}{T}}$, $A=2.3e-12, B=1765$</td>
<td>[1]</td>
</tr>
<tr>
<td>C2H6+OH→CH3CHO+0.5*CH3COO</td>
<td>$Ae^{-\frac{B}{T}}$, $A=7.9e-12, B=1030$</td>
<td>[1]</td>
</tr>
<tr>
<td>NC4H10+OH→0.9<em>CH3COE+0.1</em>CH3CHO+0.1<em>CH3COO+0.9</em>CH3CHO</td>
<td>$troe(7e-29,0.3,1.9e-12,0.0,0.7)$</td>
<td>[1], n9</td>
</tr>
<tr>
<td>C2H4+OH+M→2<em>CH3CHO+0.5</em>HO2</td>
<td>$troe(8e-27,0.3,5.3e-11,0.0,0.5)$</td>
<td>[1], n9</td>
</tr>
<tr>
<td>OXYL+OH→MEMALD+MGLYOX+0.5*oRO2</td>
<td>$1.37e-11$</td>
<td>[5]</td>
</tr>
<tr>
<td>C5H8+OH→0.32<em>MAC+0.42</em>MVK+0.74*HCHO+obio</td>
<td>$Ae^{-\frac{B}{T}}$, $A=2.55e-11, B=410$</td>
<td>[1]</td>
</tr>
<tr>
<td>APINEn+OH→0.8<em>CH3CHO+0.8</em>CH3COE+obio</td>
<td>$Ae^{-\frac{B}{T}}$, $A=1.21e-11, B=444$</td>
<td>[17]</td>
</tr>
<tr>
<td>BPINEn+OH→0.8<em>CH3CHO+0.8</em>CH3COE+obio</td>
<td>$Ae^{-\frac{B}{T}}$, $A=1.21e-11, B=444$</td>
<td>[17]</td>
</tr>
<tr>
<td>LIMONE+OH→0.8<em>CH3CHO+0.8</em>CH3COE+obio</td>
<td>$Ae^{-\frac{B}{T}}$, $A=1.21e-11, B=444$</td>
<td>[17]</td>
</tr>
<tr>
<td>HUMULE+OH→0.8<em>CH3CHO+0.8</em>CH3COE+obio</td>
<td>$Ae^{-\frac{B}{T}}$, $A=1.21e-11, B=444$</td>
<td>[17]</td>
</tr>
<tr>
<td>OCIMEN+OH→0.8<em>CH3CHO+0.8</em>CH3COE+obio</td>
<td>$Ae^{-\frac{B}{T}}$, $A=1.21e-11, B=444$</td>
<td>[17]</td>
</tr>
<tr>
<td>TERPEn+OH→0.8<em>CH3CHO+0.8</em>CH3COE+obio</td>
<td>$Ae^{-\frac{B}{T}}$, $A=1.21e-11, B=444$</td>
<td>[17]</td>
</tr>
</tbody>
</table>

### OH attack to carbonyls and peroxides

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Kinetic constants</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>HCHO+OH→CO+H2O</td>
<td>$Ae^{-\frac{B}{T}}$, $A=8.6e-12, B=20$</td>
<td>[1]</td>
</tr>
<tr>
<td>CH3CHO+OH→CH3COO</td>
<td>$Ae^{-\frac{B}{T}}$, $A=5.6e-12, B=310$</td>
<td>[1]</td>
</tr>
<tr>
<td>MEMALD+OH→GLYOX+MGLYOX+0.5*oRO2</td>
<td>$5.6e-11$</td>
<td>[1]</td>
</tr>
<tr>
<td>CH3COE+OH→CH3COYO+0.5*oRO2</td>
<td>$Ae^{-\frac{B}{T}}(300/T)^{17}$, $A=2.92e-13, B=-414, N=-2$</td>
<td>[1]</td>
</tr>
<tr>
<td>GLYOX+OH→2*CO+H2O</td>
<td>$1.1e-11$</td>
<td>[1]</td>
</tr>
<tr>
<td>MGLYOX+OH→CH3COO+CO</td>
<td>$1.5e-11$</td>
<td>[1]</td>
</tr>
<tr>
<td>MVK+OH→0.266<em>MGLYOX+0.684</em>CH3CHO+0.684<em>CH3COO+0.05</em>ISNI+0.95*oRO2</td>
<td>$Ae^{-\frac{B}{T}}, A=4.1e-12, B=453$</td>
<td>[6]</td>
</tr>
<tr>
<td>MAC+OH→0.5<em>CH3COE+0.5</em>CO2+0.5*oPAN</td>
<td>$Ae^{-\frac{B}{T}}, A=1.86e-11, B=175$</td>
<td>[6]</td>
</tr>
<tr>
<td>CH3O2H+OH→CH3O</td>
<td>$Ae^{-\frac{B}{T}}, A=1.9e-12, B=190$</td>
<td>n2</td>
</tr>
<tr>
<td>PPA+OH→CH3COO</td>
<td>$Ae^{-\frac{B}{T}}, A=1.9e-12, B=190$</td>
<td>n2</td>
</tr>
<tr>
<td>CH3O2H+OH→HCHO+O2</td>
<td>$Ae^{-\frac{B}{T}}, A=1.9e-12, B=190$</td>
<td>n2</td>
</tr>
<tr>
<td>oROOH+OH→0.8<em>OH+0.2</em>oRO2</td>
<td>$Ae^{-\frac{B}{T}}, A=3.5e-12, B=455$</td>
<td>n2</td>
</tr>
<tr>
<td>obioH+OH→OH</td>
<td>$8e-11$</td>
<td>n2</td>
</tr>
<tr>
<td>PANH+OH→0.2*oPAN</td>
<td>$1.6e-11$</td>
<td>n2</td>
</tr>
<tr>
<td>CARNIT+OH→CH3CHO+CO+N2O</td>
<td>$k(T)=Ae^{-\frac{B}{T}}, A=5.6e-12, B=-310$</td>
<td></td>
</tr>
</tbody>
</table>

### NO3 attack to hydrocarbons and aldehydes

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Kinetic constants</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH2H4+NO3→0.5<em>CARNIT+HCHO+0.5</em>oRO2</td>
<td>$2e-16$</td>
<td>[1]</td>
</tr>
<tr>
<td>C3H6+NO3→0.5<em>CARNIT+1.5</em>HCHO+0.5<em>CH3CHO+0.5</em>HO2</td>
<td>$9.45e-15$</td>
<td>[1]</td>
</tr>
<tr>
<td>APINEn+NO3→CH3CHO+CH3COE+0.5*oRO2</td>
<td>$Ae^{-\frac{B}{T}}, A=1.19e-12, B=490$</td>
<td>[8]</td>
</tr>
<tr>
<td>BPINEn+NO3→CH3CHO+CH3COE+0.5*oRO2</td>
<td>$Ae^{-\frac{B}{T}}, A=1.19e-12, B=490$</td>
<td>[8]</td>
</tr>
<tr>
<td>LIMONE+NO3→CH3CHO+CH3COE+0.5*oRO2</td>
<td>$Ae^{-\frac{B}{T}}, A=1.19e-12, B=490$</td>
<td>[8]</td>
</tr>
<tr>
<td>OCIMEN+NO3→CH3CHO+CH3COE+0.5*oRO2</td>
<td>$Ae^{-\frac{B}{T}}, A=1.19e-12, B=490$</td>
<td>[8]</td>
</tr>
<tr>
<td>HUMULE+NO3→CH3CHO+CH3COE+0.5*oRO2</td>
<td>$Ae^{-\frac{B}{T}}, A=1.19e-12, B=490$</td>
<td>[8]</td>
</tr>
<tr>
<td>TERPEn+NO3→CH3CHO+CH3COE+0.5*oRO2</td>
<td>$Ae^{-\frac{B}{T}}, A=1.19e-12, B=490$</td>
<td>[8]</td>
</tr>
<tr>
<td>C5H8+NO3→0.85<em>ISNI+0.1</em>MAC+0.05<em>MVK+0.15</em>HCHO+0.8*HO2</td>
<td>$7.8e-13$</td>
<td>[6]</td>
</tr>
<tr>
<td>HCHO+NO3→H+NO3+H2O</td>
<td>$5.8e-16$</td>
<td>[1]</td>
</tr>
<tr>
<td>CH3CHO+NO3→CH3COO+HNO3</td>
<td>$2.8e-15$</td>
<td>[9]</td>
</tr>
<tr>
<td>CH3O2+NO3→HCHO+H2O+NO2</td>
<td>$1.2e-12$</td>
<td>[10]</td>
</tr>
<tr>
<td>CH3COO+NO3→CH3O2+NO2+CO2</td>
<td>$4e-12$</td>
<td>[10]</td>
</tr>
<tr>
<td>oRO2+NO3→NO2+H2O</td>
<td>$1.2e-12$</td>
<td>[10]</td>
</tr>
<tr>
<td>obio+NO3→NO2+H2O</td>
<td>$1.2e-12$</td>
<td>[10]</td>
</tr>
<tr>
<td>oPAN+NO3→NO2+H2O</td>
<td>$4e-12$</td>
<td>[10]</td>
</tr>
</tbody>
</table>
### O3 attack to unsaturated hydrocarbons

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Kinetic constants</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>O3 attack to unsaturated hydrocarbons</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C2H4+O3 → CHCHO+0.12<em>HO2+0.13</em>H2+0.44*CO</td>
<td>Ae^{-H/T}, A=9.1e-15, B=2580</td>
<td>[1]</td>
</tr>
<tr>
<td>C3H6+O3 → -0.53<em>HCHO+0.5</em>CH3CHO+0.31*CH3O2</td>
<td>Ae^{-H/T}, A=5.5e-15, B=1880</td>
<td>[1]</td>
</tr>
<tr>
<td>+0.28<em>HO2+0.15</em>OH+0.065<em>H2+0.4</em>CO+0.7*CH4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C5H8+O3 → -0.67<em>MAC+0.26</em>MVK+0.55<em>OH+0.07</em>CH3H6</td>
<td>Ae^{-H/T}, A=1.2e-14, B=2013</td>
<td>[6]</td>
</tr>
<tr>
<td>+0.8<em>CH3O +0.06</em>HO2+0.05<em>CO+0.3</em>O3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>MAC+O3 → -0.8<em>MGLYOX+0.7</em>HCHO+0.215<em>OH+0.275</em>HO2+0.28*HO2</td>
<td>Ae^{-H/T}, A=5.3e-15, B=2520</td>
<td>[6]</td>
</tr>
<tr>
<td>+0.2<em>CO+0.2</em>O3</td>
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<td></td>
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<tr>
<td>MVK+O3 → -0.82<em>MGLYOX+0.8</em>HCHO+0.04*CH3CHO</td>
<td>Ae^{-H/T}, A=4.3e-15, B=2016</td>
<td>[6]</td>
</tr>
<tr>
<td>+0.08<em>OH+0.06</em>HO2+0.05<em>CO+0.2</em>O3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>APINEN+O3 → -1.27<em>CH3CHO+0.53</em>CH3COE+0.14*CO</td>
<td>Ae^{-H/T}, A=1.0e-15, B=736</td>
<td>[8]</td>
</tr>
<tr>
<td>+0.62<em>RO2+0.42</em>HCHO+0.85<em>OH+0.1</em>HO2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>BPINEN+O3 → -1.27<em>CH3CHO+0.53</em>CH3COE+0.14*CO</td>
<td>Ae^{-H/T}, A=1.0e-15, B=736</td>
<td>[8]</td>
</tr>
<tr>
<td>+0.62<em>RO2+0.42</em>HCHO+0.85<em>OH+0.1</em>HO2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>LIMONE+O3 → -1.27<em>CH3CHO+0.53</em>CH3COE+0.14*CO</td>
<td>Ae^{-H/T}, A=1.0e-15, B=736</td>
<td>[8]</td>
</tr>
<tr>
<td>+0.62<em>RO2+0.42</em>HCHO+0.85<em>OH+0.1</em>HO2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>TERPEN+O3 → -1.27<em>CH3CHO+0.53</em>CH3COE+0.14*CO</td>
<td>Ae^{-H/T}, A=1.0e-15, B=736</td>
<td>[8]</td>
</tr>
<tr>
<td>+0.62<em>RO2+0.42</em>HCHO+0.85<em>OH+0.1</em>HO2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>OCIMEN+O3 → -1.27<em>CH3CHO+0.53</em>CH3COE+0.14*CO</td>
<td>Ae^{-H/T}, A=1.0e-15, B=736</td>
<td>[8]</td>
</tr>
<tr>
<td>+0.62<em>RO2+0.42</em>HCHO+0.85<em>OH+0.1</em>HO2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HUMULE+O3 → -1.27<em>CH3CHO+0.53</em>CH3COE+0.14*CO</td>
<td>Ae^{-H/T}, A=1.0e-15, B=736</td>
<td>[8]</td>
</tr>
<tr>
<td>+0.62<em>RO2+0.42</em>HCHO+0.85<em>OH+0.1</em>HO2</td>
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</tbody>
</table>

### organic radical conversion

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Kinetic constants</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH3O2+NO → HCHO+NO2+HO2</td>
<td>Ae^{-H/T}, A=4.2e-12, B=-180</td>
<td>[1]</td>
</tr>
<tr>
<td>CH3COO+NO → CH3O2+NO2+CO2</td>
<td>2e-11</td>
<td></td>
</tr>
<tr>
<td>oRO2+NO → NO2+HO2</td>
<td>4e-12</td>
<td>n3</td>
</tr>
<tr>
<td>obio+NO → 0.86<em>NO2+0.78</em>HO2+0.14*ISNI</td>
<td>Ae^{-H/T}, A=1.4e-11, B=180</td>
<td>[6]</td>
</tr>
<tr>
<td>oPAN+NO → NO2+HO2</td>
<td>1.4e-11</td>
<td>n3</td>
</tr>
<tr>
<td>oRN1+NO → 1.5*NO2</td>
<td>4e-11</td>
<td>n3</td>
</tr>
</tbody>
</table>

### organic radical recombination

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Kinetic constants</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH3O2+HO2 → CH3O2H</td>
<td>Ae^{-H/T}, A=4.1e-13, B=-790</td>
<td>[1]</td>
</tr>
<tr>
<td>CH3COO+HO2 → -0.67<em>PPA+0.33</em>O3</td>
<td>Ae^{-H/T}, A=4.3e-13, B=-1040</td>
<td>[1]</td>
</tr>
<tr>
<td>oRO2+HO2 → oROOH</td>
<td>Ae^{-H/T}, A=2.7e-13, B=-1000</td>
<td>n4</td>
</tr>
<tr>
<td>obio+HO2 → obioH</td>
<td>Ae^{-H/T}, A=2.7e-13, B=-1000</td>
<td>n4</td>
</tr>
<tr>
<td>oPAN+HO2 → PANH</td>
<td>Ae^{-H/T}, A=2.7e-13, B=-1000</td>
<td>n4</td>
</tr>
<tr>
<td>oRN1+HO2 → X</td>
<td>Ae^{-H/T}, A=2.7e-13, B=-1000</td>
<td>n4</td>
</tr>
<tr>
<td>CH3O2+CH3O2 → -1.35<em>HCHO+0.7</em>HO2</td>
<td>Ae^{-H/T}, A=1.13e-13, B=-356</td>
<td>[1], n5</td>
</tr>
<tr>
<td>CH3COO+CH3O2 → -0.5<em>CH3O2+0.5</em>CO2+HCHO+0.5*HO2</td>
<td>Ae^{-H/T}, A=3.34e-12, B=-400</td>
<td>[1], n5</td>
</tr>
<tr>
<td>oRO2+CH3O2 → -0.65<em>HCHO+0.8</em>HO2+0.35*CH3OH</td>
<td>Ae^{-H/T}, A=1.5e-13, B=-220</td>
<td>n5</td>
</tr>
<tr>
<td>obio+CH3O2 → -0.8<em>HO2+0.5</em>HCHO</td>
<td>Ae^{-H/T}, A=2.44e-11, B=-223</td>
<td>n5</td>
</tr>
<tr>
<td>oPAN+CH3O2 → HCHO+0.5*HO2</td>
<td>Ae^{-H/T}, A=7.9e-12, B=-140</td>
<td>n5</td>
</tr>
<tr>
<td>CH3COO+CH3COO → -2.*CH3O2+2.*CO2</td>
<td>Ae^{-H/T}, A=2.8e-12, B=-530</td>
<td>[1], n5</td>
</tr>
<tr>
<td>oRO2+CH3COO → -0.8<em>CH3O2+0.8</em>CO2+0.8*HO2</td>
<td>Ae^{-H/T}, A=8.6e-13, B=-260</td>
<td>n5</td>
</tr>
<tr>
<td>obio+CH3COO → -0.5<em>HCHO+1.5</em>HO2+0.7*CO2</td>
<td>Ae^{-H/T}, A=1.18e-11, B=127</td>
<td>n5</td>
</tr>
<tr>
<td>oPAN+CH3COO → CH3O2+CO2+HO2</td>
<td>Ae^{-H/T}, A=3.34e-12, B=-400</td>
<td>n5</td>
</tr>
<tr>
<td>oRO2+oRO2 → -1.3*HO2</td>
<td>6.4e-14</td>
<td>n5</td>
</tr>
</tbody>
</table>
### Organic nitrates and pernitrates

<table>
<thead>
<tr>
<th>Reactions</th>
<th>Kinetic constants</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH$_3$COO$+$NO$_2$$+$$M$$\rightarrow$$PAN$ troe(2.7e-28,0,7.1,1.2e-11,0,0,9,0,3)</td>
<td>[1], n9</td>
<td></td>
</tr>
<tr>
<td>oPAN$+$NO$_2$$+$$M$$\rightarrow$$oPAN$ troe(2.7e-28,0,7.1,1.2e-11,0,0,9,0,3)</td>
<td>[6], n9</td>
<td></td>
</tr>
<tr>
<td>PAN$+$$M$$\rightarrow$$CH$_3$COO$+$NO$_2$ troe(4.9e-3,12100,0,5.4e16,13830,0,0,3)</td>
<td>[1], n9</td>
<td></td>
</tr>
<tr>
<td>oPAN$+$$M$$\rightarrow$$oPAN$ troe(4.9e-3,12100,0,5.4e16,13830,0,0,3)</td>
<td>[6], n9</td>
<td></td>
</tr>
<tr>
<td>PAN$+$OH$\rightarrow$$HCHO$+NO$_3$$+$$CO$_2$ $Ac$$^{-B/T}$,A=9.5e-13,B=650</td>
<td>[1]</td>
<td></td>
</tr>
<tr>
<td>oPAN$+$OH$\rightarrow$$oPAN$ troe(4.9e-3,12100,0,5.4e16,13830,0,0,3)</td>
<td>[6]</td>
<td></td>
</tr>
<tr>
<td>PAN$+$OH$\rightarrow$$CH$_3$COO$+$NO$_2$ troe(2.7e-28,0,7.1,1.2e-11,0,0,9,0,3)</td>
<td>[1], n9</td>
<td></td>
</tr>
<tr>
<td>oPAN$+$OH$\rightarrow$$oPAN$ troe(2.7e-28,0,7.1,1.2e-11,0,0,9,0,3)</td>
<td>[6], n9</td>
<td></td>
</tr>
</tbody>
</table>

ISNI$+$OH$\rightarrow$$0.95$$*$$CH$_3$CHO$+$$0.475$$*$$CH$_3$COE$+$$0.475$$*$$MGLYOX$$+$$0.05$$*$$ISNI$$+$$0.05$$*$$HO$_2$$+$$oRN$_1$ $3.4e$-11 | [6] |       |

### Photolytic reactions

<table>
<thead>
<tr>
<th>Reactions</th>
<th>Photorate</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>O$_3$$\rightarrow$$2$$*$OH</td>
<td>photorate</td>
<td>[3], n7</td>
</tr>
<tr>
<td>NO$_2$$\rightarrow$$NO$$+$$O$_3$</td>
<td>photorate</td>
<td>[3]</td>
</tr>
<tr>
<td>NO$_3$$\rightarrow$$NO$$+$$O$_3$</td>
<td>photorate</td>
<td>[3], [11]</td>
</tr>
<tr>
<td>N$_2$O$_5$$\rightarrow$$NO$$+$$O$_3$</td>
<td>photorate</td>
<td>[3]</td>
</tr>
<tr>
<td>H$_2$O$_2$$\rightarrow$$2$$*$OH</td>
<td>photorate</td>
<td>[3]</td>
</tr>
<tr>
<td>HNO$_3$$\rightarrow$$NO$$+$$O$_3$</td>
<td>photorate</td>
<td>[3]</td>
</tr>
<tr>
<td>HONO$\rightarrow$$OH$$+$$HO$_2$</td>
<td>photorate</td>
<td>[3]</td>
</tr>
<tr>
<td>oROOH$\rightarrow$$OH$$+$$HO$_2$</td>
<td>photorate</td>
<td>[3]</td>
</tr>
<tr>
<td>PANH$\rightarrow$$OH$$+$$HO$_2$</td>
<td>photorate</td>
<td>n8</td>
</tr>
<tr>
<td>PAN$+$CH$_3$COO$+$$NO$_2$</td>
<td>photorate</td>
<td>[3]</td>
</tr>
</tbody>
</table>

- [1] Atkinson et al., 1997
- [2] Donahue et al., 1997
- [6] Paulson and Seinfeld, 1992
- [8] Atkinson et al., 1994
- [9] DeMore et al., 1990
- [10] Canosa-Mas et al., 1996
- [14] Plum et al., 1983
- [15] Bierbach et al., 1994
- [16] Lightfoot et al., 1996
- [17] Kirchner and Stockwell, 1996
- [18] Aumont, 2002

- **n1**: Rate constants containing a density dependent term in a minor reaction channel have been simplified by putting an average boundary layer molecular density of 2.5*10$^{19}$ molecules/cm$^3$.

- **n2**: For operator reactions with OH, oROOH is interpreted as 2-butyl hydrogen peroxide, obioH as a peroxide from isoprene degradation, PANH represents unsaturated organic peroxides; due to lack of data, the rate constants of these compounds and of peroxy acetyl acid have been estimated using structure reactivity relationships in Kwok and Atkinson (1995).

- **n3**: The rate constant of the operator reaction oRO2$+$$NO$ has been set to that of the i-C$_3$H$_7$O$_2$$+$$NO$
reaction given in [16], that of oPAN+NO to that of CH3COO2+NO [1], the rate constant for oRO2NO+NO is taken from that of ISNIR (nitrate peroxy radicals from isoprene degradation) + NO

n4 : The rate constants for the operator reactions oRO2, obio, RO2NI+HO2 have been set to that of reaction C2H5O2+HO2 [1], that of oPAN+HO2 has been taken from CH3COO2+HO2 [1].

n5 : Radical conserving and terminating pathways are combined to single reactions; rate constants in operator reactions are affected by interpreting oRO2 as 2-butyl peroxy radical [16], obio as a peroxy radical from isoprene degradation [6] and oPAN as CH3COO2.

n6 : Reaction rates of the operators oPAN and OPAN have been set to those of the peroxy acetyl radical and PAN, respectively.

n7 : The reactions O3+hv→O(1D), O(1D)+H2O→2OH, O(1D)+M→O(3P)+M and O(3P)+O2+M→O3+M have been combined to reaction O3+hv→O(1D) by taking into account H2O and M concentrations in order to adjust the photolysis frequency.

n8 : Due to lack of data, photolysis frequencies of higher organic peroxides are taken as that of CH3OOH.

n9 : Three body Troe reactions [1], given in the form:

\[ k = \frac{k_0[M]}{1 + \frac{k_0[M]}{k_\infty}} \]

with

\[ Z = \frac{1}{1 + \left( \log_{10} \left( \frac{k_0(T)[M]}{k_\infty(T)} \right) \right)^2} \]

\[ k_0 = A_0 e^{-\frac{B_0}{T}} \left( \frac{T}{300} \right)^{-n}, \text{ and } k_\infty = A_\infty e^{-\frac{B_\infty}{T}} \left( \frac{T}{300} \right)^{-m}, \]

The parameters are given in the order \(A_0, B_0, n, A_\infty, B_\infty, m, f\).

### 10.2.4 Species list of the SAPRC-07-A gas-phase chemical mechanism

<table>
<thead>
<tr>
<th><strong>Species</strong></th>
<th><strong>Definition</strong></th>
<th><strong>lumped class</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Inorganic compounds</td>
<td></td>
<td></td>
</tr>
<tr>
<td>O3</td>
<td>ozone</td>
<td>APINEN</td>
</tr>
<tr>
<td>H2O2</td>
<td>hydrogen peroxide</td>
<td>BPINEN</td>
</tr>
<tr>
<td>OH</td>
<td>hydroxy radical</td>
<td>LIMONE</td>
</tr>
<tr>
<td>HO2</td>
<td>hydroperoxy radical</td>
<td></td>
</tr>
<tr>
<td>NO</td>
<td>nitric oxide</td>
<td></td>
</tr>
<tr>
<td>NO2</td>
<td>nitrogen dioxide</td>
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</tr>
<tr>
<td>NO3</td>
<td>nitrogen trioxide</td>
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<td>N2O5</td>
<td>dinitrogen pentoxide</td>
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<td>HNO3</td>
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<td>CO</td>
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<td>SO2</td>
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<tr>
<td>BENZ</td>
<td>benzene</td>
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<tr>
<td>C5H8</td>
<td>isoprene</td>
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<td>AFG1</td>
<td>lumped photoreactive monounsaturated dicarbonyl aromatic fragmentation products that photolyze to form radicals</td>
<td></td>
</tr>
<tr>
<td>AFG2</td>
<td>lumped photoreactive monounsaturated dicarbonyl aromatic fragmentation products that photolyze to form non-radical products</td>
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</tbody>
</table>
Aumont et al. (1997)

### Inorganic chemistry

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Kinetic constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>O₃+NO→NO₂</td>
<td>k(T) = (Ae^{-B/B/T}), A=3.00e-12, B=1500</td>
</tr>
<tr>
<td>O₃+NO₂→NO₃</td>
<td>k(T) = (Ae^{-B/B/T}), A=1.40e-13, B=2470</td>
</tr>
<tr>
<td>NO+NO₃→2NO₂</td>
<td>k(T) = (Ae^{-B/B/T}), A=1.80e-11, B=110</td>
</tr>
<tr>
<td>NO₂+NO₂→2NO₂</td>
<td>k(T) = (Ae^{-B/B/T}), A=3.30e-39, B=530</td>
</tr>
<tr>
<td>NO₂+NO₃+M→N₂O₅</td>
<td>k(T,M) = saprc_troe(3.60e-30,-460,1.40e-2199,6.50e-34,-B/T,0.10,11080,0.35,1.33)</td>
</tr>
<tr>
<td>N₂O₅+M→NO₂+NO₃</td>
<td>k(T,M) = saprc_troe(1.30e-03,3.50,11000,9.70e+14,0.10,11080,0.35,1.33)</td>
</tr>
<tr>
<td>N₂O₅+H₂O→2H₂O₃</td>
<td>k=2.50e-22</td>
</tr>
<tr>
<td>N₂O₅+H₂O+H₂O→2H₂O₃</td>
<td>k=1.80e-39</td>
</tr>
<tr>
<td>NO₂+NO₃→NO₂+NO₂</td>
<td>k(T,M) = saprc_troe(7.00e-31,-2.60e-0,3.60e-11,-0.10,0.60,1.0)</td>
</tr>
<tr>
<td>OH+NO+M→HONO</td>
<td>k(T,M) = saprc_troe(1.80e-30,-3.00e-110,0.0,0.60,1.0)</td>
</tr>
<tr>
<td>OH+HONO→NO₂</td>
<td>k=2.00e-11</td>
</tr>
<tr>
<td>OH+NO₂+M→HNO₃</td>
<td>k(T) = saprc_2(2.40e-14,-460,2.70e-17,-2199,6.50e-34,-1335)</td>
</tr>
<tr>
<td>OH+NO₃→HO₂+NO₂</td>
<td>k(T) = saprc_1(1.44e-13,0.3,43e-33,0.)</td>
</tr>
<tr>
<td>OH+O₃→HO₂</td>
<td>k(T) = (Ae^{-B/B/T}), A=1.70e-12, B=940</td>
</tr>
<tr>
<td>HO₂+NO→OH+NO₂</td>
<td>k(T) = (Ae^{-B/B/T}), A=3.60e-12, B=270</td>
</tr>
<tr>
<td>HO₂+NO₂+M→HNO₄</td>
<td>k(T,M) = saprc_troe(2.00e-31,-3.40e-0,2.90e-12,-1.10,0.60,1.0)</td>
</tr>
</tbody>
</table>

¹For the concept of “chemical operators” see Carter (1990) and Aumont et al. (1997)

### Organic peroxides

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Kinetic constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>XOOH → Lumped organic hydroperoxide structure, used to represent the effect of photolysis of the hydroperoxide group in the SAPRC-99 peroxy radical representation (Carter, 2000).</td>
<td></td>
</tr>
<tr>
<td>COOH → Methyl Hydroperoxide</td>
<td></td>
</tr>
<tr>
<td>FACD → Formic Acid</td>
<td></td>
</tr>
<tr>
<td>PACD → Higher organic acids</td>
<td></td>
</tr>
<tr>
<td>AACD → Acetic Acid</td>
<td></td>
</tr>
</tbody>
</table>

### Peroxy radicals

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Kinetic constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>TBUO → t-Butoxy radicals</td>
<td></td>
</tr>
<tr>
<td>RCO₃ → Peroxy Propionyl and higher peroxy acyl Radicals</td>
<td></td>
</tr>
<tr>
<td>MEO₂ → Acetyl Peroxy Radicals</td>
<td></td>
</tr>
<tr>
<td>MACO₃ → Peroxyacyl radicals formed from methacrolein and other acroleins</td>
<td></td>
</tr>
<tr>
<td>BZCO₃ → Peroxyacetyl radical formed from Aromatic Aldehydes</td>
<td></td>
</tr>
<tr>
<td>BZO → Phenoxy Radicals</td>
<td></td>
</tr>
</tbody>
</table>

### Operators

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Kinetic constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>R2O2 → Peroxy Radical Operator representing NO consumption with organic nitrate formation</td>
<td></td>
</tr>
<tr>
<td>R2O → Peroxy Radical Operator representing NO to NO₂ conversion with HO₂ formation</td>
<td></td>
</tr>
<tr>
<td>R2O₂ → Peroxy Radical Operator representing NO to NO₂ conversion without HO₂ formation</td>
<td></td>
</tr>
</tbody>
</table>

---

HO + NO₂ → N₂O₅

HO2NO3+M→N2O5

NO→NO₂

NO₂→NO₃

CO→CO₂

CCHO→Acetone

CRES→Phenols and Cresols

CRES→Phenols and Cresols

MACR→Methacrolein

MAPAN→PAN analogues formed from Methacrolein

RCHO→Lumped C3+ Aldehydes

RCO3→Peroxy Acetyl Nitrate

RO3→Lumped Organic Nitrates

RO→Lumped Organic Nitrates

RO₂R→Peroxy Radical Operator representing NO to NO₂

RO₂N→Peroxy Radical Operator representing NO consumption

RCO₃→Peroxyacyl radicals formed from acroleins

MACO₃→Peroxyacyl radicals formed from methacrolein and other acroleins

MECO₃→Peroxyacyl radicals formed from Aromatic Aldehydes

BZO→Phenoxy Radicals

XOOH→Lumped organic hydroperoxide structure, used to represent the effect of photolysis of the hydroperoxide group in the SAPRC-99 peroxy radical representation (Carter, 2000).

COOH→Methyl Hydroperoxide

FACD→Formic Acid

PACD→Higher organic acids

AACD→Acetic Acid

TBUO→t-Butoxy Radicals

RCO₃→Peroxy Propionyl and higher peroxy acyl Radicals

MEO₂→Acetyl Peroxy Radicals

MACO₃→Peroxyacyl radicals formed from methacrolein and other acroleins

BZCO₃→Peroxyacetyl radical formed from Aromatic Aldehydes

BZO→Phenoxy Radicals

RO₂N→Peroxy Radical Operator representing NO consumption

RO→Peroxy Radical Operator representing NO to NO₂ conversion without HO₂ formation

RO₂→Peroxy Radical Operator representing NO to NO₂ conversion with HO₂ formation

---

**Reaction list of the SAPRC-07-A chemical mechanism**
<table>
<thead>
<tr>
<th>Reactions</th>
<th>Kinetic constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>HNO₄+M→HO₂+NO₂</td>
<td>k(T,M)=saprc_troe(3.72e-05,2.40,10650,5.42e+15,2.30,11170,0.60,1.0)</td>
</tr>
<tr>
<td>HNO₄+OH→NO₂</td>
<td>k(T)=Ae⁻⁹¹/T,A=1.30e-12,B=-380</td>
</tr>
<tr>
<td>HO₂+O₃→OH</td>
<td>k(T)=Ae⁻⁹¹/(300/T)²,A=2.03e-16,B=693,N=4.57</td>
</tr>
<tr>
<td>HO₂+HO₂→H₂O₂</td>
<td>k(T)=saprc₁(2.20e-13,-600,1.90e-33,-980)</td>
</tr>
<tr>
<td>HO₂+H₂O₂→H₂O</td>
<td>k(4.00e-12)</td>
</tr>
<tr>
<td>NO₃+NO₃→2*NO₂</td>
<td>k(T)=Ae⁻⁹¹/T,A=8.50e-13,B=2450</td>
</tr>
<tr>
<td>H₂O₂+OH→H₂O</td>
<td>k=1.80e-12</td>
</tr>
<tr>
<td>OH+H₂O₂→H₂O</td>
<td>k(T)=Ae⁻⁹¹/T,A=4.80e-11,B=-250</td>
</tr>
<tr>
<td>OH+H₂O→H₂O</td>
<td>k(T)=Ae⁻⁹¹/T,A=7.70e-12,B=2100</td>
</tr>
<tr>
<td>SOₓ chemistry</td>
<td></td>
</tr>
<tr>
<td>OH+SO₂+M→H₂O₂+H₂SO₄</td>
<td>k(T,M)=saprc_troe(3.30e-31,-4.30,0.,1.60e-12,0.,0.,0.60,1.0)</td>
</tr>
<tr>
<td>RO₂X operator</td>
<td></td>
</tr>
<tr>
<td>RO₂R+NO→NO₂+HO₂</td>
<td>k(T)=Ae⁻⁹¹/T,A=2.60e-12,B=380</td>
</tr>
<tr>
<td>RO₂R+HO₂→XOH</td>
<td>k(T)=Ae⁻⁹¹/T,A=3.80e-13,B=900</td>
</tr>
<tr>
<td>RO₂R+NO₃→NO₂+HO₂</td>
<td>k=2.30e-12</td>
</tr>
<tr>
<td>RO₂R+MEO₂→HO₂+0.75<em>HCHO+0.25</em>MEOH</td>
<td>k(T)=Ae⁻⁹¹/T,A=3.80e-13,B=900</td>
</tr>
<tr>
<td>RO₂R+RO₂R→HO₂</td>
<td>k=3.50e-14</td>
</tr>
<tr>
<td>RO₂N+NO→RNNO₃</td>
<td>k(T)=Ae⁻⁹¹/T,A=2.60e-12,B=380</td>
</tr>
<tr>
<td>RO₂N+HO₂→XOH+PRD₂</td>
<td>k(T)=Ae⁻⁹¹/T,A=3.80e-13,B=900</td>
</tr>
<tr>
<td>RO₂N+NO₃→NO₂+HO₂+PRD₂</td>
<td>k(2.30e-12)</td>
</tr>
<tr>
<td>RO₂N+MEO₂→HO₂+0.25<em>MEOH+PRD₂+0.75</em>HCHO</td>
<td>k=2e-13</td>
</tr>
<tr>
<td>RO₂N+RO₂R→HO₂+PRD₂</td>
<td>k=3.50e-14</td>
</tr>
<tr>
<td>RO₂N+RO₂N→HO₂+2*PRD₂</td>
<td>k=3.50e-14</td>
</tr>
<tr>
<td>MECO₃+RO₂R→MEO₂+CO₂</td>
<td>k(T)=Ae⁻⁹¹/T,A=4.40e-13,B=1070</td>
</tr>
<tr>
<td>MECO₃+RO₂N→MEO₂+CO₂+HO₂+PRD₂</td>
<td>k(T)=Ae⁻⁹¹/T,A=4.40e-13,B=1070</td>
</tr>
<tr>
<td>MACO₃+RO₂R→CO₂+HCHO+MECO₃</td>
<td>k(T)=Ae⁻⁹¹/T,A=4.40e-13,B=1070</td>
</tr>
<tr>
<td>MACO₃+RO₂N→CO₂+HCHO+MECO₃+HO₂+PRD₂</td>
<td>k(T)=Ae⁻⁹¹/T,A=4.40e-13,B=1070</td>
</tr>
<tr>
<td>R₂O₂+RO₂R→RO₂R</td>
<td>k=3.50e-14</td>
</tr>
<tr>
<td>R₂O₂+RO₂N→RO₂N</td>
<td>k=3.50e-14</td>
</tr>
<tr>
<td>R₂O₂+R₂O₂→X</td>
<td>k=3.50e-14</td>
</tr>
<tr>
<td>R₂O₂+MECO₃→MECO₃</td>
<td>k(T)=Ae⁻⁹¹/T,A=4.40e-13,B=1070</td>
</tr>
<tr>
<td>R₂O₂+RCO₃→RCO₃</td>
<td>k(T)=Ae⁻⁹¹/T,A=4.40e-13,B=1070</td>
</tr>
<tr>
<td>R₂O₂+BZCO₃→BZCO₃</td>
<td>k(T)=Ae⁻⁹¹/T,A=4.40e-13,B=1070</td>
</tr>
<tr>
<td>R₂O₂+MACO₃→MACO₃</td>
<td>k(T)=Ae⁻⁹¹/T,A=4.40e-13,B=1070</td>
</tr>
<tr>
<td>R₂O₂+R₂O₂→R₂O₂</td>
<td>k(T)=Ae⁻⁹¹/T,A=4.40e-13,B=1070</td>
</tr>
<tr>
<td>R₂O₂+MACO₃→MACO₃</td>
<td>k(T)=Ae⁻⁹¹/T,A=4.40e-13,B=1070</td>
</tr>
<tr>
<td>R₂O₂+R₂O₂→R₂O₂+R₂O₂+X</td>
<td>k(T)=Ae⁻⁹¹/T,A=4.40e-13,B=1070</td>
</tr>
<tr>
<td>OH attack to hydrocarbons</td>
<td></td>
</tr>
<tr>
<td>AFG1+OH→0.521<em>RO₂R+0.201</em>MECO₃+0.217<em>MACO₃+0.06</em>RO₂N+0.202<em>R₂O₂+0.334</em>CO+0.407<em>RCHO+0.129</em>MEK+0.107<em>GLY+0.267</em>MGLY+0.284*XC</td>
<td>k=7.40e-11</td>
</tr>
<tr>
<td>AFG₂+OH→0.521<em>RO₂R+0.201</em>MECO₃+0.217<em>MACO₃+0.06</em>RO₂N+0.202<em>R₂O₂+0.334</em>CO+0.407<em>RCHO+0.129</em>MEK+0.107<em>GLY+0.267</em>MGLY+0.284*XC</td>
<td>k=7.40e-11</td>
</tr>
<tr>
<td>AFG₃+OH→0.561<em>RO₂R+0.117</em>MECO₃+0.206<em>MACO₃+0.117</em>RO₂N+0.172<em>R₂O₂+0.114</em>CO+0.274<em>GLY+0.153</em>MGLY+0.019<em>BAACL+0.231</em>IPRD+0.195<em>AFG1+0.195</em>AFG2+0.938*XC</td>
<td>k=9.35e-11</td>
</tr>
<tr>
<td>CH₄+OH→MEO₂</td>
<td>k(T)=Ae⁻⁹¹/T,A=1.85e-12,B=1690</td>
</tr>
<tr>
<td>C₂H₄+OH+M→R₂O₂+1.61<em>HCHO+0.195</em>CCHO</td>
<td>k(T,M)=saprc_troe(1.00e-28,-4.50,0.,8.80e-12,-0.85,0.,0.60,1.0)</td>
</tr>
<tr>
<td>C₅H₈+OH→0.907<em>RO₂R+0.093</em>RO₂N+0.079<em>R₂O₂+0.624</em>HCHO+0.23<em>MACR+0.32</em>MVK+0.357<em>IPRD+0.167</em>XC</td>
<td>k(T)=Ae⁻⁹¹/T,A=2.54e-11,B=410</td>
</tr>
</tbody>
</table>
### OH attack to carbonyls and peroxides

<table>
<thead>
<tr>
<th>Reactions</th>
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</tr>
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<tbody>
<tr>
<td>ACYE+OH+M→0.3<em>HO2+0.7</em>OH+0.3<em>CO+0.3</em>FACD+0.7*GLY</td>
<td>k(T,M)=sapre_trct(5.50e-30,-2.000,0.8,30e-13,0.0,0.0,60,1.0)</td>
</tr>
<tr>
<td>BENZ+OH→0.57<em>HO2+0.29</em>RO2R+0.116<em>OH+0.024</em>RO2N</td>
<td>k(T)=Ae^{-B/T},A=2.33e-12,B=193</td>
</tr>
<tr>
<td>+0.29<em>GLY+0.57</em>CRES+0.029<em>AFG1+0.261</em>AFG2+0.116<em>AFG3+0.976</em>XC</td>
<td></td>
</tr>
<tr>
<td>ALK1+OH→RO2R+CCHO</td>
<td>k(T)=Ae^{-B/T}(300/T)^N,N=1.34e-12,B=499,N=2</td>
</tr>
<tr>
<td>ALK2+OH→0.965<em>RO2R+0.305</em>RO2N+0.261<em>RCHO+0.704</em>ACET+0.105*XC</td>
<td>k(T)=Ae^{-B/T}(300/T)^N,N=1.49e-12,B=87,N=2</td>
</tr>
<tr>
<td>ALK3+OH→0.695<em>RO2R+0.236</em>TBUO+0.07<em>RO2N+0.558</em>RO2O</td>
<td>k(T)=Ae^{-B/T},A=1.51e-12,B=126</td>
</tr>
<tr>
<td>+0.026<em>HCHO+0.445</em>CCHO+0.122<em>RCHO+0.024</em>ACET+0.332<em>MEK+0.046</em>XC</td>
<td></td>
</tr>
<tr>
<td>ALK4+OH→0.83<em>RO2R+0.011</em>MEO2+0.011<em>MEC03+0.149</em>RO2N</td>
<td>k(T)=Ae^{-B/T},A=3.75e-12,B=44</td>
</tr>
<tr>
<td>+0.933<em>RO2R+0.002</em>CO+0.029<em>HCHO+0.438</em>CCHO+0.236*RCHO</td>
<td></td>
</tr>
<tr>
<td>+0.426<em>ACET+0.106</em>MEK+0.146<em>PRD2+0.119</em>XC</td>
<td></td>
</tr>
<tr>
<td>ALK5+OH→0.647<em>RO2R+0.353</em>RO2N+0.958<em>RO2O+0.04</em>HCHO</td>
<td>k(T)=Ae^{-B/T},A=2.70e-12,B=374</td>
</tr>
<tr>
<td>+0.106<em>CCHO+0.209</em>RCHO+0.071<em>ACET+0.086</em>MEK</td>
<td></td>
</tr>
<tr>
<td>+0.407<em>PRD2+0.204</em>XC</td>
<td></td>
</tr>
<tr>
<td>OLE1+OH→0.904<em>RO2R+0.001</em>MEO2+0.005<em>RO2N+0.234</em>RO2O</td>
<td>k(T)=Ae^{-B/T},A=6.18e-12,B=501</td>
</tr>
<tr>
<td>+0.7<em>HCHO+0.301</em>CCHO+0.47<em>RCHO+0.005</em>ACET+0.119*PRD2</td>
<td></td>
</tr>
<tr>
<td>+0.026<em>MACR+0.008</em>MVK+0.006<em>IPRD+0.822</em>XC</td>
<td></td>
</tr>
<tr>
<td>OLE2+OH→0.914<em>RO2R+0.086</em>RO2N+0.052<em>RO2O+0.209</em>HCHO</td>
<td>k(T)=Ae^{-B/T},A=1.26e-11,B=488</td>
</tr>
<tr>
<td>+0.788<em>CCHO+0.481</em>RCHO+0.136<em>ACET+0.076</em>MEK+0.022*PRD2</td>
<td></td>
</tr>
<tr>
<td>+0.027<em>MACR+0.002</em>MVK+0.037<em>IPRD+0.111</em>XC</td>
<td></td>
</tr>
<tr>
<td>ARO1+OH→0.166<em>HO2+0.482</em>RO2R+0.284<em>OH+0.068</em>RO2N</td>
<td>k=6.15e-12</td>
</tr>
<tr>
<td>+0.077<em>PRD2+0.218</em>GLY+0.138<em>MGLY+0.166</em>CRES+0.049*BALD</td>
<td></td>
</tr>
<tr>
<td>+0.164<em>AFG1+0.193</em>AFG2+0.284<em>AFG3+0.002</em>XC</td>
<td></td>
</tr>
<tr>
<td>ARO2+OH→0.018<em>HO2+0.58</em>RO2R+0.02<em>OH+0.11</em>RO2N</td>
<td>k=2.57e-11</td>
</tr>
<tr>
<td>+0.035<em>PRD2+0.116</em>GLY+0.286<em>MGLY+0.104</em>BACL+0.108*CRES</td>
<td></td>
</tr>
<tr>
<td>+0.039<em>BALD+0.217</em>AFG1+0.21<em>AFG2+0.282</em>AFG3+1.486*XC</td>
<td></td>
</tr>
<tr>
<td>GLY+OH→0.63<em>HO2+0.37</em>RCO3+1.26<em>CO+0.37</em>XC</td>
<td>k=1.10e-11</td>
</tr>
<tr>
<td>MGLY+OH→MECO3+CO</td>
<td>k=1.50e-11</td>
</tr>
<tr>
<td>CRES+OH→0.8<em>RO2R+0.2</em>BZO+0.25<em>MGLY+5.05</em>XC</td>
<td>k(T)=Ae^{-B/T},A=1.70e-12,B=950</td>
</tr>
<tr>
<td>NPHE+OH→BZO+XN</td>
<td>k=3.50e-12</td>
</tr>
<tr>
<td>BALD+OH→BZCO3</td>
<td>k=1.20e-11</td>
</tr>
<tr>
<td>MACR+OH→0.5<em>RO2R+0.5</em>MACO3+0.416<em>CO+0.084</em>HCHO</td>
<td>k(T)=Ae^{-B/T},A=8.00e-12,B=380</td>
</tr>
<tr>
<td>+0.416<em>MEK+0.084</em>MGLY+0.416*XC</td>
<td></td>
</tr>
<tr>
<td>MVK+OH→0.3<em>RO2R+0.675</em>MECO3+0.025<em>RO2N+0.675</em>RO2O</td>
<td>k(T)=Ae^{-B/T},A=2.60e-12,B=610</td>
</tr>
<tr>
<td>+0.3<em>HCHO+0.675</em>RCHO+0.3<em>MGLY+0.725</em>XC</td>
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</tr>
<tr>
<td>IPRD+OH→0.67<em>RO2R+0.289</em>MACO3+0.041<em>RO2N+0.336</em>CO</td>
<td>k=6.19e-11</td>
</tr>
<tr>
<td>+0.055<em>HCHO+0.129</em>CCHO+0.013<em>RCHO+0.15</em>MEK+0.332*PRD2</td>
<td></td>
</tr>
<tr>
<td>+0.15<em>GLY+0.174</em>MGLY+0.504*XC</td>
<td></td>
</tr>
<tr>
<td>PRD2+OH→0.472<em>HO2+0.379</em>RO2R+0.029<em>MECO3+0.049</em>RCO3</td>
<td>k=1.55e-11</td>
</tr>
<tr>
<td>+0.071<em>RO2N+0.094</em>RO2R+0.213<em>HCHO+0.084</em>CHOO+0.545*RCHO</td>
<td></td>
</tr>
<tr>
<td>+0.115<em>MEK+0.336</em>PRD2+0.877*XC</td>
<td></td>
</tr>
<tr>
<td>MEOH+OH→HO2+HCHO</td>
<td>k(T)=Ae^{-B/T},A=2.85e-12,B=345</td>
</tr>
<tr>
<td>FACD+OH→HO2+CO2</td>
<td>k=4.50e-13</td>
</tr>
<tr>
<td>AACD+OH→0.491<em>RO2R+0.509</em>MEO2+0.509<em>CO2+0.491</em>MGLY+0.491*XC</td>
<td>k(T)=Ae^{-B/T},A=4.20e-14,B=855</td>
</tr>
<tr>
<td>PACD+OH→RO2R+0.143<em>CO2+0.142</em>CCHO+0.4*RCHO</td>
<td>k=1.20e-12</td>
</tr>
<tr>
<td>+0.457<em>BACL+0.455</em>XC</td>
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<tr>
<td>COOH+OH→0.3<em>OH+0.7</em>MEO2+0.3*HCHO</td>
<td>k(T)=Ae^{-B/T},A=3.80e-12,B=200</td>
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<tr>
<td>ACET+OH→MECO3+RO22+HCHO</td>
<td>k(T)=Ae^{-B/T}(300/T)^N,N=4.56e-14,B=429,N=-3.65</td>
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<tr>
<td>RCHO+OH→0.035<em>RO2R+0.965</em>RCO3+0.035<em>CO+0.035</em>CCHO</td>
<td>k(T)=Ae^{-B/T},A=4.4e-12,B=365</td>
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<tr>
<td>CCHO+OH→MECO3</td>
<td>k(T)=Ae^{-B/T},A=5.4e-12,B=135</td>
</tr>
<tr>
<td>HCHO+OH→HO2+CO</td>
<td>k(T)=Ae^{-B/T}(300/T)^N,N=1.3e-12,B=25,N=2</td>
</tr>
<tr>
<td>MEK+OH→0.376<em>RO2R+0.51</em>MECO3+0.074<em>RCO3+0.039</em>RO2N</td>
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</table>
## Reactions Kinetic constants

**organic nitrates and pernitrates**

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Kinetic constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>RNO3+OH→−0.189<em>H2O+0.305</em>R2O2+0.332<em>NO2+0.175</em>R2ON+0.671<em>R2O2+0.011</em>HCHO+0.429<em>CCHO+0.037</em>RCHO+0.004<em>ACET+0.18</em>MEKO+0.039<em>PRD2+0.494</em>RNO3+0.174<em>XN+0.04</em>XC</td>
<td>k=7.20e-12</td>
</tr>
<tr>
<td>PAN+M→MEO3+NO2</td>
<td>k(T)=saprc_troe(4.90e-03,0.12100,0.400e+16.0,1.36000,0.30,1.41)</td>
</tr>
<tr>
<td>PAN2→RCO3+NO2</td>
<td>k(T)=Ac−B/T, A=8.30e+16, B=13940</td>
</tr>
<tr>
<td>PBZM→BZC30+NO2</td>
<td>k(T)=Ac−B/T, A=7.90e+16, B=14000</td>
</tr>
<tr>
<td>MAPAN→MAC30+NO2</td>
<td>k(T)=Ac−B/T, A=1.6e+16, B=13486</td>
</tr>
<tr>
<td>MAC30+NO2→PAN</td>
<td>k(T)=Ac−B/T, A=2.3e+11, B=−150</td>
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**NO3 attack**

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Kinetic constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>MEO2+NO3→HCHO+H2O2+NO2</td>
<td>k=1.00e-13</td>
</tr>
<tr>
<td>MECO3+NO3→MEO2+CO2+NO2</td>
<td>k=2.3e-12</td>
</tr>
<tr>
<td>RCO3+NO3→NO2+CO2+BZO+R2O2</td>
<td>k=2.3e-12</td>
</tr>
<tr>
<td>MACO3+NO3→NO2+CO2+HCHO+MECO3</td>
<td>k=2.3e-12</td>
</tr>
<tr>
<td>R2O3+NO3→NO2</td>
<td>k=2.3e-12</td>
</tr>
<tr>
<td>HCHO+NO3→HNO3+HO2+CO</td>
<td>k(T)=Ac−B/T, A=1.40e−12, B=1895</td>
</tr>
<tr>
<td>CCHO+NO3→MECO3+HNO3</td>
<td>k(T)=Ac−B/T, A=8.20e−12, B=2376</td>
</tr>
<tr>
<td>RCCHO+NO3→RCO3+HNO3</td>
<td>k(T)=Ac−B/T, A=1.40e−12, B=2431</td>
</tr>
<tr>
<td>GLY+NO3→0.63<em>H2O+0.37</em>RCO3+HNO3+1.26<em>CO+0.37</em>XC</td>
<td>k(T)=Ac−B/T, A=1.40e−12, B=2431</td>
</tr>
<tr>
<td>MACR+NO3→0.5<em>RO2R+0.5</em>MACO3+0.5<em>HNO3+0.5</em>CO+0.5<em>XN+1.5</em>XC</td>
<td>k(T)=Ac−B/T, A=1.34e−12, B=1860</td>
</tr>
<tr>
<td>IPRD+NO3→0.799<em>RO2R+0.176</em>RO2N+0.009<em>RCO3+0.009</em>MECO3+0.009<em>CO+0.009</em>HCHO+0.009<em>MGLY+0.009</em>ACET+0.009<em>ACF+0.009</em>MVK+0.009<em>IPRD+0.009</em>XN</td>
<td>k(T)=Ac−B/T, A=1.50e−12, B=1815</td>
</tr>
<tr>
<td>C2H4+NO3→RO2R+RCHO+XN+1.5*XC</td>
<td>k(T)=Ac−B/T, A=2.00e−13, B=382</td>
</tr>
<tr>
<td>OLE1+NO3→RO2R+RCHO+XN+1.5*XC</td>
<td>k(T)=Ac−B/T, A=2.00e−13, B=382</td>
</tr>
<tr>
<td>OLE2+NO3→RO2R+RCHO+XN+1.5*XC</td>
<td>k(T)=Ac−B/T, A=2.00e−13, B=382</td>
</tr>
<tr>
<td>AFG1+O3→−0.522<em>H2O+0.826</em>OH+0.652<em>RCO3+0.652</em>R2O2+0.522<em>CO+0.174</em>CO2+0.652<em>HCHO+0.432</em>GLY+0.568<em>MGLY+0.872</em>XC</td>
<td>k(T)=Ac−B/T, A=3.30e−12, B=2880, N=2</td>
</tr>
<tr>
<td>AFG2+O3→−0.522<em>H2O+0.826</em>OH+0.652<em>RCO3+0.652</em>R2O2+0.522<em>CO+0.174</em>CO2+0.652<em>HCHO+0.432</em>GLY+0.568<em>MGLY+0.872</em>XC</td>
<td>k(T)=Ac−B/T, A=9.66e−18</td>
</tr>
<tr>
<td>AFG3+O3→−0.522<em>H2O+0.826</em>OH+0.652<em>RCO3+0.652</em>R2O2+0.522<em>CO+0.174</em>CO2+0.652<em>HCHO+0.432</em>GLY+0.568<em>MGLY+0.872</em>XC</td>
<td>k(T)=Ac−B/T, A=9.66e−18</td>
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**Ozonolysis**

<table>
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<tr>
<th>Reaction</th>
<th>Kinetic constants</th>
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<tr>
<td>AFG1+O3→−0.522<em>H2O+0.826</em>OH+0.652<em>RCO3+0.652</em>R2O2+0.522<em>CO+0.174</em>CO2+0.652<em>HCHO+0.432</em>GLY+0.568<em>MGLY+0.872</em>XC</td>
<td>k(T)=Ac−B/T, A=9.66e−18</td>
</tr>
<tr>
<td>AFG2+O3→−0.522<em>H2O+0.826</em>OH+0.652<em>RCO3+0.652</em>R2O2+0.522<em>CO+0.174</em>CO2+0.652<em>HCHO+0.432</em>GLY+0.568<em>MGLY+0.872</em>XC</td>
<td>k(T)=Ac−B/T, A=9.66e−18</td>
</tr>
<tr>
<td>AFG3+O3→−0.522<em>H2O+0.826</em>OH+0.652<em>RCO3+0.652</em>R2O2+0.522<em>CO+0.174</em>CO2+0.652<em>HCHO+0.432</em>GLY+0.568<em>MGLY+0.872</em>XC</td>
<td>k(T)=Ac−B/T, A=1.43e−17</td>
</tr>
<tr>
<td>AFG4+O3→−0.522<em>H2O+0.826</em>OH+0.652<em>RCO3+0.652</em>R2O2+0.522<em>CO+0.174</em>CO2+0.652<em>HCHO+0.432</em>GLY+0.568<em>MGLY+0.872</em>XC</td>
<td>k(T)=Ac−B/T, A=1.43e−17</td>
</tr>
<tr>
<td>AFG5+O3→−0.522<em>H2O+0.826</em>OH+0.652<em>RCO3+0.652</em>R2O2+0.522<em>CO+0.174</em>CO2+0.652<em>HCHO+0.432</em>GLY+0.568<em>MGLY+0.872</em>XC</td>
<td>k(T)=Ac−B/T, A=1.43e−17</td>
</tr>
<tr>
<td>AFG6+O3→−0.522<em>H2O+0.826</em>OH+0.652<em>RCO3+0.652</em>R2O2+0.522<em>CO+0.174</em>CO2+0.652<em>HCHO+0.432</em>GLY+0.568<em>MGLY+0.872</em>XC</td>
<td>k(T)=Ac−B/T, A=1.43e−17</td>
</tr>
<tr>
<td>AFG7+O3→−0.522<em>H2O+0.826</em>OH+0.652<em>RCO3+0.652</em>R2O2+0.522<em>CO+0.174</em>CO2+0.652<em>HCHO+0.432</em>GLY+0.568<em>MGLY+0.872</em>XC</td>
<td>k(T)=Ac−B/T, A=1.43e−17</td>
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</tbody>
</table>
Reactions

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Kinetic Constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>IPRD+O₃→−0.4<em>HO₂+0.285</em>OH+0.048<em>RCO₃+0.048</em>R₂O₂</td>
<td>k=4.18e-18</td>
</tr>
<tr>
<td>+0.498<em>CO+0.14</em>R₂O₂+0.125<em>HCHO+0.047</em>CCHO+0.21*MEK</td>
<td></td>
</tr>
<tr>
<td>+0.14<em>FACD+0.372</em>PACD+0.023<em>GLY+0.742</em>MGLY+0.329*X</td>
<td></td>
</tr>
<tr>
<td>C₂H₄+O₃→→−0.16<em>HO₂+0.16</em>OH+0.51<em>CO+0.12</em>CO₂+HCHO</td>
<td></td>
</tr>
<tr>
<td>+0.37*FACD</td>
<td></td>
</tr>
<tr>
<td>ACRY+O₃→→−1.5<em>HO₂+0.55</em>OH+1.5<em>CO+0.5</em>CO₂</td>
<td></td>
</tr>
<tr>
<td>OLE₁+O₃→→−0.116<em>HO₂+0.04</em>RO₂R+0.193<em>OH+0.104</em>MEO₂</td>
<td></td>
</tr>
<tr>
<td>+0.004<em>RO₂N+0.023</em>R₂O₂+0.368<em>CO₂+0.125</em>CO₂+0.5*HCHO</td>
<td></td>
</tr>
<tr>
<td>+0.154<em>CCHO+0.384</em>RCHO+0.002<em>ACET+0.006</em>MEK+0.189*PRD₂</td>
<td></td>
</tr>
<tr>
<td>+0.185<em>FACD+0.022</em>AACD+0.112<em>PACD+0.69</em>XC</td>
<td></td>
</tr>
<tr>
<td>OLE₂+O₃→→−0.093<em>HO₂+0.039</em>RO₂R+0.423<em>OH+0.29</em>MEO₂</td>
<td></td>
</tr>
<tr>
<td>+0.14<em>MECO₃+0.008</em>RCO₃+0.003<em>RO₂N+0.161</em>R₂O₂+0.297*CO</td>
<td></td>
</tr>
<tr>
<td>+0.162<em>CO₂+0.26</em>HCHO+0.495<em>CCHO+0.333</em>RCHO+0.048*ACET</td>
<td></td>
</tr>
<tr>
<td>+0.032<em>MEK+0.042</em>PRD₂+0.033<em>FACD+0.061</em>AACD+0.222<em>PACD+0.028</em>MACR+0.021<em>MK+0.125</em>XC</td>
<td></td>
</tr>
<tr>
<td>MACR+O₃→→−0.108<em>HO₂+0.208</em>OH+0.15<em>RCO₃+0.15</em>R₂O₂</td>
<td></td>
</tr>
<tr>
<td>+0.45<em>CO+0.117</em>CO₂+0.2<em>HCHO+0.333</em>FACD+0.9<em>MGLY+0.1</em>XC</td>
<td></td>
</tr>
</tbody>
</table>

**organic radical conversion**

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Kinetic Constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>MEO₂+NO→→→NO₂+HCHO+HO₂</td>
<td>k(T)=Ae⁻²(B/T), A=2.30e-12, B=360</td>
</tr>
<tr>
<td>MECO₃+NO→→→NO₂+CO₂+NO₂</td>
<td>k(T)=Ae⁻²(B/T), A=7.50e-12, B=290</td>
</tr>
<tr>
<td>RCO₂+NO→→→NO₂+CHOO+RO₂R+CO₂</td>
<td>k(T)=Ae⁻²(B/T), A=6.70e-12, B=340</td>
</tr>
<tr>
<td>BZO₂+NO→→→NO₂+CO₂+BO₂+R₂O₂</td>
<td>k(T)=Ae⁻²(B/T), A=6.70e-12, B=340</td>
</tr>
<tr>
<td>MACO₃+NO→→→NO₂+CO₂+HCHO+MECO₃</td>
<td>k(T)=Ae⁻²(B/T), A=6.70e-12, B=340</td>
</tr>
<tr>
<td>R₂O₂+NO→NO₂</td>
<td>k(T)=Ae⁻²(B/T), A=2.6e-12, B=380</td>
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</table>

**organic radical recombinasion**

<table>
<thead>
<tr>
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<th>Kinetic Constants</th>
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</thead>
<tbody>
<tr>
<td>MEO₂+HO₂→→→COOH</td>
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</tr>
<tr>
<td>MEO₂+H₂O→→→HCHO</td>
<td></td>
</tr>
<tr>
<td>MEO₂+MEO₂→→→MEOH+HCHO</td>
<td></td>
</tr>
<tr>
<td>MEO₂+MEO₂→→→2<em>HCHO+2</em>HO₂</td>
<td></td>
</tr>
<tr>
<td>MECO₃+H₂O→→→AACD+0.3*O³</td>
<td></td>
</tr>
<tr>
<td>MECO₃+MEO₂+0.1<em>AACD+0.1</em>HCHO+0.9<em>HCHO+0.9</em>HO₂+0.9<em>MEO₂+0.9</em>CO₂</td>
<td></td>
</tr>
<tr>
<td>MECO₃+MECO₃→→→2<em>MEO₂+2</em>CO₂</td>
<td></td>
</tr>
<tr>
<td>RCO₂+HO₂→→→PACD+0.25*O³</td>
<td></td>
</tr>
<tr>
<td>RCO₂+MEO₂→→→CO₂+RO₂R+CHOO+HCHO+HO₂</td>
<td></td>
</tr>
<tr>
<td>RCO₂+MEO₂+2<em>CO₂+MEO₂+2</em>CHOO+RO₂R+H₂O</td>
<td></td>
</tr>
<tr>
<td>RCO₂+RCO₂+2<em>CHOO+2</em>RO₂R+2*CO₂</td>
<td></td>
</tr>
<tr>
<td>BZO₂+H₂O→→→PACD+0.25<em>O³+4</em>XC</td>
<td></td>
</tr>
<tr>
<td>BZO₂+MEO₂→→→CO₂+BZO₂+R₂O₂+HCHO+HO₂</td>
<td></td>
</tr>
<tr>
<td>BZO₂+MECO₂→→→2*CO₂+MECO₂+BZO₂+R₂O₂</td>
<td></td>
</tr>
<tr>
<td>BZO₂+R₂O₂→→→2*CO₂+CCHOO+R₂O₂+R₂O₂+BZO₂</td>
<td></td>
</tr>
<tr>
<td>BZO₂+BCO₂→→→2<em>BO₂+2</em>R₂O₂+2*CO₂</td>
<td></td>
</tr>
<tr>
<td>MACO₂+H₂O→→→PACD+0.25<em>O³+4</em>XC</td>
<td></td>
</tr>
<tr>
<td>MACO₂+MEO₂+2<em>HCHO+2</em>HO₂+MECO₃</td>
<td></td>
</tr>
<tr>
<td>MACO₂+MECO₃→→→2*CO₂+MECO₂+HCHO+MECO₃</td>
<td></td>
</tr>
<tr>
<td>MACO₂+RCO₂→→→HCHO+MECO₃+CHOO+RO₂R+2*CO₂</td>
<td></td>
</tr>
<tr>
<td>MACO₂+BCO₂→→→HCHO+MECO₃+BZO₂+R₂O₂+2*CO₂</td>
<td></td>
</tr>
<tr>
<td>MACO₂+MACO₂→→→2<em>HCHO+2</em>MECO₂+2*CO₂</td>
<td></td>
</tr>
<tr>
<td>BZO₂+H₂O→→→CRES+1*XC</td>
<td></td>
</tr>
<tr>
<td>R₂O₂+H₂O→→→HO₂</td>
<td></td>
</tr>
<tr>
<td>R₂O₂+MEO₂→→→MEO₂</td>
<td>k=2e-13</td>
</tr>
<tr>
<td>BZO→→→CRES+2RO₂+1*XC</td>
<td>k=1e-3</td>
</tr>
<tr>
<td>TBÜO→→→ACET+MEO₂</td>
<td>k(T)=Ae⁻²(B/T), A=7.5e+14, B=8152</td>
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**photolytic reactions**

<table>
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<tr>
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<th>Kinetic Constants</th>
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<tr>
<td>NO₂→NO+O₃</td>
<td>J(Z)=photorate(NO₂)</td>
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<tr>
<td>NO→NO</td>
<td>J(Z)=photorate(NO₃-1)</td>
</tr>
<tr>
<td>Reactions</td>
<td>Kinetic constants</td>
</tr>
<tr>
<td>-----------</td>
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</tr>
<tr>
<td>NO₃→NO₂+O₃</td>
<td>J(Z)=photorate(NO₃-2)</td>
</tr>
<tr>
<td>O₃→2*OH</td>
<td>J(T,Z,H₂O)=photorate(O₃-1)</td>
</tr>
<tr>
<td>HONO→OH+NO</td>
<td>J(Z)=photorate(HONO)</td>
</tr>
<tr>
<td>HNO₃→OH+NO₂</td>
<td>J(Z)=photorate(HNO₃)</td>
</tr>
<tr>
<td>HNO₄→0.61<em>HO₂+0.61</em>NO₂+0.39<em>OH+0.39</em>NO₃</td>
<td>J(Z)=photorate(HNO₄)</td>
</tr>
<tr>
<td>H₂O₂→2*OH</td>
<td>J(Z)=photorate(H₂O₂)</td>
</tr>
<tr>
<td>PAN→0.6<em>MECO₃+0.6</em>NO₂+0.4<em>CO₂+0.4</em>NO3</td>
<td>J(Z)=photorate(PAN)</td>
</tr>
<tr>
<td>PAN→0.6<em>R₂O₂+0.4</em>CO₂+0.4<em>CHOO+0.4</em>RO₂R+0.4<em>CO₂+0.4</em>NO₃</td>
<td>J(Z)=photorate(PAN2)</td>
</tr>
<tr>
<td>PBZN→0.6<em>BZCO₃+0.6</em>NO₂+0.4<em>CO₂+0.4</em>R₂O₂+0.4<em>RO₂R+0.4</em>NO₃</td>
<td>J(Z)=photorate(PBZN)</td>
</tr>
<tr>
<td>MAPAN→0.6<em>MACO₃+0.6</em>NO₂+0.4<em>CO₂+0.4</em>HCHO+0.4<em>MECO₃+0.4</em>NO₃</td>
<td>J(Z)=photorate(MAPAN)</td>
</tr>
<tr>
<td>HCHO→2*HO₂+CO</td>
<td>J(Z)=photorate(HCHO-1)</td>
</tr>
<tr>
<td>HCHO→CO</td>
<td>J(Z)=photorate(HCHO-2)</td>
</tr>
<tr>
<td>CCHO→HO₂+MECO₃+CO⁺CHCO</td>
<td>J(Z)=photorate(CCHO)</td>
</tr>
<tr>
<td>ACET→1.38<em>MEO₂+0.62</em>MECO₃+0.38*CO</td>
<td>J(Z)=photorate(ACET)</td>
</tr>
<tr>
<td>MEK→R₂O₂⁺MECO₃+CHCO</td>
<td>J(Z)=photorate(MEK)</td>
</tr>
<tr>
<td>HO₂→0.61<em>HO₂+0.61</em>MECO₃+0.39<em>CO₂+0.39</em>NO₃</td>
<td>J(Z)=photorate(HO₂)</td>
</tr>
<tr>
<td>C₅H₈+O₃→0.066<em>HO₂+0.266</em>OH+0.192<em>MACO₃+0.008</em>RO₂N+0.192<em>RO₂R+0.257</em>CO⁺0.122<em>CO₂+0.592</em>HCHO+0.1<em>PRD₂⁺0.204</em>FACD⁺0.39<em>MACR⁺0.16</em>MVK⁺0.15<em>IPRD⁺0.559</em>XC</td>
<td>k(T)=Ac⁻¹/T, A=7.86e⁻¹5, B=1912</td>
</tr>
<tr>
<td>C₅H₈+NO₃→0.749<em>RO₂R+0.187</em>NO₂+0.064<em>RO₂N+1.347</em>R₂O₂⁺0.042<em>R₂O₂⁺0.042</em>RO₂N⁺0.388<em>R₂O₂⁺0.001</em>CO⁺0.264<em>HCHO⁺0.533</em>RCHO⁺0.036<em>ACET⁺0.005</em>MEK⁺0.255<em>PRD₂⁺0.009</em>MGLY⁺0.014<em>MACR⁺0.007</em>BACL⁺0.005<em>MVK⁺0.001</em>MACR⁺0.001<em>IPRD⁺0.001</em>PRD₂⁺0.056*XC</td>
<td>k(T)=Ac⁻¹/T, A=3.03e⁻¹2, B=448</td>
</tr>
<tr>
<td>C₅H₈+OH→0.759<em>RO₂R⁺0.042</em>R₂O₂⁺0.042<em>RO₂N⁺0.388</em>R₂O₂⁺0.001<em>CO⁺0.264</em>HCHO⁺0.533<em>RCHO⁺0.036</em>ACET⁺0.005<em>MEK⁺0.255</em>PRD₂⁺0.009<em>MGLY⁺0.014</em>BACL⁺0.005<em>MVK⁺0.001</em>MACR⁺0.001<em>IPRD⁺0.001</em>PRD₂⁺0.056*XC</td>
<td>k(T)=Ac⁻¹/T, A=3.03e⁻¹2, B=448</td>
</tr>
<tr>
<td>TERPEN+OH→0.759<em>RO₂R⁺0.042</em>R₂O₂⁺0.042<em>RO₂N⁺0.388</em>R₂O₂⁺0.001<em>CO⁺0.264</em>HCHO⁺0.533<em>RCHO⁺0.036</em>ACET⁺0.005<em>MEK⁺0.255</em>PRD₂⁺0.009<em>MGLY⁺0.014</em>BACL⁺0.005<em>MVK⁺0.001</em>MACR⁺0.001<em>IPRD⁺0.001</em>PRD₂⁺0.056*XC</td>
<td>k(T)=Ac⁻¹/T, A=3.03e⁻¹2, B=448</td>
</tr>
<tr>
<td>TERPEN+O₃→0.052<em>HO₂+0.067</em>RO₂R+0.585<em>OH+0.126</em>MACO₃+0.149<em>R₂O₂+0.203</em>RO₂N+0.808<em>RO₂N+0.185</em>CO⁺0.045<em>CO₂⁺0.229</em>HCHO⁺0.22<em>RCHO⁺0.165</em>ACET⁺0.004<em>MEK⁺0.409</em>PRD₂⁺0.107<em>MACR⁺0.001</em>FACD⁺0.001<em>Gly⁺0.002</em>MGLY⁺0.005<em>BACL⁺0.001</em>MACR⁺0.001<em>IPRD⁺0.432</em>MVK⁺0.001<em>MACR⁺0.001</em>IPRD⁺0.432<em>R₂O₂⁺0.001</em>MACR⁺0.001<em>IPRD⁺0.432</em>XC</td>
<td>k(T)=Ac⁻¹/T, A=9.57e⁻¹6, B=785</td>
</tr>
<tr>
<td>TERPEN+NO₃→RO₂R+0.421<em>NO₂⁺0.019</em>R₂O₂⁺0.397<em>RO₂N⁺1.347</em>R₂O₂⁺0.01<em>CO⁺0.017</em>HCHO⁺0.001<em>CCHO⁺0.509</em>RCHO⁺0.175<em>ACET⁺0.001</em>MGLY⁺0.007<em>MACR⁺0.001</em>MVK⁺0.002<em>PRD₂⁺0.163</em>R₂O₂⁺0.416<em>XN⁺4.473</em>XC</td>
<td>k(T)=Ac⁻¹/T, A=1.28e⁻¹2, B=490</td>
</tr>
<tr>
<td>Reactions</td>
<td>Kinetic constants</td>
</tr>
<tr>
<td>---------------------------------</td>
<td>----------------------------------------</td>
</tr>
<tr>
<td>APINEN+OH—0.759<em>RO2R+0.042</em>RCO3+0.2<em>RO2N+0.388</em>R2O2 +0.001<em>CO+0.264</em>HCHO+0.533<em>RCOO+0.036</em>ACET+0.005<em>MEK +0.255</em>PRD2+0.009<em>MGLY+0.014</em>BACL+0.002<em>MVK +0.001</em>IPRD+5.056*XC</td>
<td>( k(T)=Ae^{-B/T} ), ( A=1.87e-11, B=-435 )</td>
</tr>
<tr>
<td>APINEN+O3—0.052<em>HO2+0.067</em>RO2R+0.858<em>OH+0.126</em>MECO3 +0.149<em>RCO3+0.203</em>RO2N+0.808<em>R2O2+0.185</em>CO+0.045<em>CO2 +0.229</em>HCHO+0.22<em>RCHO+0.165</em>ACET+0.004<em>MEK+0.409</em>PRD2 +0.107<em>FACD+0.043</em>PACD+0.001<em>GLY+0.002</em>MGLY+0.055<em>BACL +0.001</em>MACR+0.001<em>IPRD+3.526</em>XC</td>
<td>( k(T)=Ae^{-B/T} ), ( A=9.57e-16, B=785 )</td>
</tr>
<tr>
<td>APINEN+NO3—0.162<em>RO2R+0.421</em>NO2+0.019<em>RCO3+0.397</em>RO2N +1.347<em>R2O2+0.01</em>CO+0.17<em>HCHO+0.001</em>CCHO+0.509<em>RCHO +0.175</em>ACET+0.001<em>MGLY+0.003</em>MACR+0.001<em>MVK+0.002</em>IPRD +0.163<em>RNO3+0.416</em>XN+4.473*XC</td>
<td>( k(T)=Ae^{-B/T} ), ( A=1.28e-12, B=-490 )</td>
</tr>
<tr>
<td>BPINEN+OH—0.759<em>RO2R+0.042</em>RCO3+0.2<em>RO2N+0.388</em>R2O2 +0.001<em>CO+0.264</em>HCHO+0.533<em>RCOO+0.036</em>ACET+0.005<em>MEK +0.255</em>PRD2+0.009<em>MGLY+0.014</em>BACL+0.002<em>MVK +0.001</em>IPRD+5.056*XC</td>
<td>( k(T)=Ae^{-B/T} ), ( A=9.57e-16, B=785 )</td>
</tr>
<tr>
<td>BPINEN+O3—0.052<em>HO2+0.067</em>RO2R+0.858<em>OH+0.126</em>MECO3 +0.149<em>RCO3+0.203</em>RO2N+0.808<em>R2O2+0.185</em>CO+0.045<em>CO2 +0.229</em>HCHO+0.22<em>RCHO+0.165</em>ACET+0.004<em>MEK+0.409</em>PRD2 +0.107<em>FACD+0.043</em>PACD+0.001<em>GLY+0.002</em>MGLY+0.055<em>BACL +0.001</em>MACR+0.001<em>IPRD+3.526</em>XC</td>
<td>( k(T)=Ae^{-B/T} ), ( A=9.57e-16, B=785 )</td>
</tr>
<tr>
<td>BPINEN+NO3—0.162<em>RO2R+0.421</em>NO2+0.019<em>RCO3+0.397</em>RO2N +1.347<em>R2O2+0.01</em>CO+0.17<em>HCHO+0.001</em>CCHO+0.509<em>RCHO +0.175</em>ACET+0.001<em>MGLY+0.003</em>MACR+0.001<em>MVK+0.002</em>IPRD +0.163<em>RNO3+0.416</em>XN+4.473*XC</td>
<td>( k(T)=Ae^{-B/T} ), ( A=1.28e-12, B=-490 )</td>
</tr>
<tr>
<td>LIMONE+OH—0.759<em>RO2R+0.042</em>RCO3+0.2<em>RO2N+0.388</em>R2O2 +0.001<em>CO+0.264</em>HCHO+0.533<em>RCOO+0.036</em>ACET+0.005<em>MEK +0.255</em>PRD2+0.009<em>MGLY+0.014</em>BACL+0.002<em>MVK +0.001</em>IPRD+5.056*XC</td>
<td>( k(T)=Ae^{-B/T} ), ( A=9.57e-16, B=785 )</td>
</tr>
<tr>
<td>LIMONE+O3—0.052<em>HO2+0.067</em>RO2R+0.858<em>OH+0.126</em>MECO3 +0.149<em>RCO3+0.203</em>RO2N+0.808<em>R2O2+0.185</em>CO+0.045<em>CO2 +0.229</em>HCHO+0.22<em>RCHO+0.165</em>ACET+0.004<em>MEK+0.409</em>PRD2 +0.107<em>FACD+0.043</em>PACD+0.001<em>GLY+0.002</em>MGLY+0.055<em>BACL +0.001</em>MACR+0.001<em>IPRD+3.526</em>XC</td>
<td>( k(T)=Ae^{-B/T} ), ( A=9.57e-16, B=785 )</td>
</tr>
<tr>
<td>LIMONE+NO3—0.162<em>RO2R+0.421</em>NO2+0.019<em>RCO3+0.397</em>RO2N +1.347<em>R2O2+0.01</em>CO+0.17<em>HCHO+0.001</em>CCHO+0.509<em>RCHO +0.175</em>ACET+0.001<em>MGLY+0.003</em>MACR+0.001<em>MVK+0.002</em>IPRD +0.163<em>RNO3+0.416</em>XN+4.473*XC</td>
<td>( k(T)=Ae^{-B/T} ), ( A=1.28e-12, B=-490 )</td>
</tr>
<tr>
<td>OCIMEN+OH—0.759<em>RO2R+0.042</em>RCO3+0.2<em>RO2N+0.388</em>R2O2 +0.001<em>CO+0.264</em>HCHO+0.533<em>RCOO+0.036</em>ACET+0.005<em>MEK +0.255</em>PRD2+0.009<em>MGLY+0.014</em>BACL+0.002<em>MVK +0.001</em>IPRD+5.056*XC</td>
<td>( k(T)=Ae^{-B/T} ), ( A=9.57e-16, B=785 )</td>
</tr>
<tr>
<td>OCIMEN+O3—0.052<em>HO2+0.067</em>RO2R+0.858<em>OH+0.126</em>MECO3 +0.149<em>RCO3+0.203</em>RO2N+0.808<em>R2O2+0.185</em>CO+0.045<em>CO2 +0.229</em>HCHO+0.22<em>RCHO+0.165</em>ACET+0.004<em>MEK+0.409</em>PRD2 +0.107<em>FACD+0.043</em>PACD+0.001<em>GLY+0.002</em>MGLY+0.055<em>BACL +0.001</em>MACR+0.001<em>IPRD+3.526</em>XC</td>
<td>( k(T)=Ae^{-B/T} ), ( A=9.57e-16, B=785 )</td>
</tr>
<tr>
<td>OCIMEN+NO3—0.162<em>RO2R+0.421</em>NO2+0.019<em>RCO3+0.397</em>RO2N +1.347<em>R2O2+0.01</em>CO+0.17<em>HCHO+0.001</em>CCHO+0.509<em>RCHO +0.175</em>ACET+0.001<em>MGLY+0.003</em>MACR+0.001<em>MVK+0.002</em>IPRD +0.163<em>RNO3+0.416</em>XN+4.473*XC</td>
<td>( k(T)=Ae^{-B/T} ), ( A=1.28e-12, B=-490 )</td>
</tr>
<tr>
<td>HUMULE+OH—0.759<em>RO2R+0.042</em>RCO3+0.2<em>RO2N+0.388</em>R2O2 +0.001<em>CO+0.264</em>HCHO+0.533<em>RCOO+0.036</em>ACET+0.005<em>MEK +0.255</em>PRD2+0.009<em>MGLY+0.014</em>BACL+0.002<em>MVK+0.001</em>IPRD +5.056*XC</td>
<td>( k(T)=Ae^{-B/T} ), ( A=9.57e-16, B=785 )</td>
</tr>
</tbody>
</table>
Reactions Kinetic constants

HUMULE+O3→0.052*HO2+0.067*RO2R+0.585*OH+0.126*MEO3
+0.149*RCO3+0.203*RO2N+0.808*R2O2+0.185*CO2
+0.229*HCHO+0.22*RCHO+0.165*ACET+0.004*MEK+0.409*PRD2
+0.107*FACD+0.043*PACD+0.001*GLY+0.002*MGLY+0.055*BACL
+0.001*MACR+0.001*IPRD+3.526*X

k(T)=Ae^{−B/T}, A=9.57e-16, B=785

HUMULE+NO3→0.162*RO2R+0.421*NO2+0.019*RCO3+0.397*RO2N
+1.347*R2O2+0.01*CO+0.017*HCHO+0.001*CCHO+0.509*RCHO
+0.175*ACET+0.001*MGLY+0.003*MACR+0.001*MVK+0.002*IPRD
+0.163*RNO3+0.416*XN+4.473*X

k(T)=Ae^{−B/T}, A=1.28e-12, B=-490

• The reactions O3+hν→O(1D), O(1D)+H2O→2OH, O(1D)+M→O(3P)+M and O(3P)+O2→O3+M
  have been combined to reaction O3+hν→O(1D) by taking into account H2O and M concentrations in
  order to adjust the photolysis frequency.

• The reactions OH+CO→HO2+CO2, HO2+HO2→H2O2 et HO2+HO2+H2O→H2O2 :

  \[ k(T, M) = k_1(T) + k_2(T) \left[ M \right] \]

  The parameters are given in the order A_1, B_1, A_2, B_2

• The reactions OH+HNO3→NO3 :

  \[ k(T, M) = k_0(T) + \frac{k_3(T) \left[ M \right]}{1 + \frac{k_3(T) \left[ M \right]}{k_2(T)}} \]

  The parameters are given in the order A_0, B_0, A_2, B_2, A_3, B_3

• Three body Troe reactions :

  \[ k(T, M) = \frac{k_0(T) \left[ M \right]}{1 + \frac{k_0(T) \left[ M \right]}{k_\infty(T)}} \times F^Z \]

  with

  \[ Z = \frac{1}{1 + \left( \frac{\log_{10} \left( \frac{k_0(T) \left[ M \right]}{k_\infty(T)} \right)}{N} \right)^2} \]

  \[ k_0 = A_0 e^{−B_0/T} \left( \frac{T}{300} \right)^{-n}, \text{ and } k_\infty = A_\infty e^{−B_\infty/T} \left( \frac{T}{300} \right)^{-m} \]

  The parameters are given in the order A_0, n, B_0, A_\infty, m, B_\infty, F, N

10.3 Aerosol processes

10.3.1 Overview

CHIMERE consists in the baseline gas-phase version with MELCHIOR2 chemistry, together
with a sectional aerosol module. This module accounts for 7 species (primary particle material, nitrate, sulfate, ammonium,
biogenic secondary organic aerosol (SOA), anthropogenic SOA and water). Potentially, Chloride et Sodium
can be included (high computing time). In its initial version the module uses 6 bins from 10 nm to 40
µm. Physical processes into account are described below. See also sections on chemistry (aqueous-phase
chemistry, heterogenous chemistry and SOA formation) below. Dry and wet scavenging/deposition are also
described in separate sections.

The physical processes accounted for are coagulation ([Gelbard and Seinfeld, 1980]), absorption
([Nenes et al., 1998]) and nucleation ([Kulmala et al., 1998],[Kavouras et al., 1998]). See following subsections
for details.
• **Coagulation:** Classical theory already used by [Gelbard and Seinfeld, 1980].

• **Absorption:** Absorption is taken into account for both inorganic and organic species but their processing is different. For inorganic species, equilibrium concentrations are computed with the thermodynamic module ISORROPIA (or a tabulated version) presented in [Nenes et al., 1998]. For secondary organic species, equilibrium concentrations are calculated through a temperature dependent partitioning coefficient ([Pankow, 1994]). Please note that the ISORROPIA code is included in CHIMERE, please check the ISORROPIA web site for downloading the latest version.

• **Nucleation:** The parameterization of [Kulmala et al., 1998] for sulfuric acid nucleation is used. This process, favoured by cold humid atmospheric conditions, affects the number of ultrafine particles. The nucleated flux is added to the smallest bin in the sectional distribution. Although nucleation of condensable organic species has been clearly identified in many experimental studies ([Kavouras et al., 1998], there is no available parameterization. Since the sulfuric acid nucleation process competes with absorption processes, it is expected to occur in weakly particle polluted conditions.

### 10.3.2 Composition and mathematical representation of aerosols

*This section was published in [Bessagnet et al., 2005].*

Atmospheric aerosols are represented by their size distributions and compositions. The sectional representation described by [Gelbard and Seinfeld, 1980] has been used for the density distribution function. The sectional approach is quite useful to solve the governing equation for multicomponent aerosols. It discretizes the density distribution in a finite number of bins ([Warren, 1986]). Thus, all particles in section \( l \) have the same composition and are characterized by their mean diameter \( d_l \). The aerosol module actually uses six bins from 10 nm to 40 \( \mu \)m, following a geometrical progression. For a given \( x \) as \( x = \ln(m) \), with \( m \) the particle mass, \( q(x) \) is the density distribution as defined in Equation 10.3, \( Q \) being the mass concentration function. \( Q_l^k (\mu g \, m^{-3}) \) is the mass concentration of component \( k \) in section \( l \) and \( Q_l (\mu g \, m^{-3}) \) is the total mass concentration in section \( l \) (Equation 10.4).

\[
q(x) = \frac{dQ}{dx} \tag{10.3}
\]

\[
Q_l = \int_{x_{l-1}}^{x_l} q(x)dx = \sum_k Q_l^k \tag{10.4}
\]

<table>
<thead>
<tr>
<th>Model species</th>
<th>Species</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>pPPM</td>
<td>Anthropogenic primary species EC, OCp, and other industrial dusts</td>
<td>primary</td>
</tr>
<tr>
<td>pSOA</td>
<td>Anthropogenic and Biogenic secondary organic aerosol (ASOA+BSOA)</td>
<td>secondary</td>
</tr>
<tr>
<td>pH2SO4</td>
<td>Equivalent Sulfate((^\ast))</td>
<td>secondary</td>
</tr>
<tr>
<td>pHNO3</td>
<td>Equivalent Nitrate((^\ast))</td>
<td>secondary</td>
</tr>
<tr>
<td>pNH3</td>
<td>Equivalent Ammonium((^\ast))</td>
<td>primary emitted, secondary transferred</td>
</tr>
<tr>
<td>pWATER</td>
<td>Water</td>
<td></td>
</tr>
</tbody>
</table>

Table 10.4: List of aerosol species. (\(^\ast\)): ions, molecules, crystals

In the model, particles are composed of species listed in Table 10.4. Sulfate is formed through gaseous and aqueous oxidation of SO\(_2\). Nitric acid is produced in the gas phase by NO\(_x\) oxidation. N\(_2\)O\(_5\) is converted into nitric acid via heterogeneous pathways by oxidation on aqueous aerosols. Ammonia is a primary emitted base converted in the aerosol phase by neutralization with nitric and sulfuric acids. Ammonia, nitrate and sulfate exist in aqueous, gaseous and particulate phases in the model. As an example, in the particulate phase the model species pNH\(_3\) represents an equivalent ammonium as the sum of NH\(_4^+\) ion, NH\(_3\) liquid, NH\(_4\)NO\(_3\) solid, etc.
10.3.3 Coagulation

Since $Q_k^l$ is the mass concentration of component $k$ in section $l$, the mass balance equation for coagulation [Gelbard and Seinfeld, 1980] follows Equation 10.5:

$$\left[ \frac{dQ_k^l}{dt} \right]_{\text{coag}} = \frac{1}{2} \sum_{i=1}^{l-1} \sum_{j=1}^{l-1} \left[ 1^{a \beta_{i,j,l}} Q_j^l Q_i^j + 1^{b \beta_{i,j,l}} Q_i^j Q_j^i \right] - \sum_{i=1}^{l-1} \left[ 2^{a \beta_{i,l}} Q_i^l Q_i^l - 2^{b \beta_{i,l}} Q_i^l Q_i^l \right] - \frac{1}{2} \beta_{i,l} Q_i^l Q_i^l - Q_i^l \sum_{i=l+1}^m 4^{\beta_{i,l}} Q_i^l$$

Equation 10.5

The sectional coagulation coefficients $1^{a \beta}, 1^{b \beta}, 2^{a \beta}, 2^{b \beta}, 3^{\beta}$ and $4^{\beta}$ (Fuch, 1964) depend on particle characteristics and meteorological data such as temperature, pressure and turbulence parameters. For submicronic particles, coagulation is essentially driven by Brownian motions. For coarse particles sedimentation is an efficient process.

10.3.4 Absorption

The absorption flux $J$ ($\mu g m^{-3} s^{-1}$) of a semi-volatile inorganic or organic species onto a monodisperse aerosol is:

$$J = \frac{1}{\tau} (G - G_{eq})$$

with $G$ and $G_{eq} (\mu g m^{-3})$, respectively, are the gas phase and equilibrium concentrations. The characteristic time $\tau$ is:

$$\tau = \frac{1 + \frac{8 \lambda}{\pi \lambda c d N}}{2 \pi \lambda c d N}$$

Equation 10.7

with $\lambda$ (m) is the mean free path of air molecules, $d$ (m) the particle diameter, $N$ (particle m$^{-3}$) the particle number concentration, $\alpha$ the accommodation coefficient of the transferred species and $c$ (m s$^{-1}$), its mean molecular velocity. For a semi-volatile species $k$, a mean absorption coefficient $H_k^l$ (s$^{-1}$) is defined at section $l$ as:

$$\left[ \frac{dQ_k^l}{dt} \right]_{\text{abso}} = H_k^l Q_k^l$$

Equation 10.8

$$H_k^l = \frac{12 \lambda c_k}{\rho_p d_l^2 (1 + (8 \lambda / \alpha_k d_l))} (G^k - G_{eq}^k)$$

Equation 10.9

where $\rho_p$ is the particle density (fixed at 1500 kg$m^{-3}$ here). For semi-volatile inorganic species (sulfate, nitrate, ammonium), the equilibrium concentration $G_{eq}$ is calculated using the thermodynamic module ISORROPIA ([Nenes et al., 1998]). This model also determines the water content of particles. Interactions between inorganic and organic species are not taken into account, the thermodynamic of such mixtures still being poorly understood. Equilibrium concentrations for the semivolatile organic species $k$ are related to particle concentrations through a temperature dependent partition coefficient $K_p$ (in m$^3$µg$^{-1}$) ([Pankow, 1994]):

$$G_{eq}^l = \frac{Q_l^k}{OM_l K_p^k}$$

Equation 10.10
with OM (µgm⁻³) is the absorbent organic material concentration. Considering the thermodynamic equilibrium between the gas and particulate phases, this coefficient is given by

\[ K_p^k = 10^{-6} \frac{MW_{om}\zeta_k p_0^i}{R} \]  

with \( R \) is the ideal gas constant (8.206 10⁻⁵ m³ atm mol⁻¹ K⁻¹), \( T \) the temperature (K), \( MW_{om} \) the mean molecular weight (g mol⁻¹), \( p_0^i \) the vapor pressure of product \( i \) as a pure liquid (atm) and \( \zeta \) the activity coefficient of species in the bulk aerosol phase. The coefficient \( \zeta \), difficult to calculate, is assumed constant and equal to unity. Moreover, an empirical formulae can be used to estimate \( K_p^k \):

\[ \log(K_p^k) = -0.61\log(p_0^i) - 4.74 \]  

(10.12)

according to [Kaupp and Umlauf, 1992] for organic species.

### 10.3.5 Nucleation

The parameterization of [Kulmala et al., 1998] for sulfuric acid nucleation is used. This process, favoured by cold humid atmospheric conditions, affects the number of ultrafine particles. The nucleated flux is added to the smallest bin in the sectional distribution. Nucleation of condensable organic species has been clearly identified in many experimental studies ([Kavouras et al., 1998]), there is no available parameterization. Since, the sulfuric acid nucleation process competes with absorption processes, it is expected to occur in weakly particle polluted conditions.

### 10.3.6 ISORROPIA

This section is extracted from the PHD manuscript of Alma Hodzic, 2005.

The inorganic part mainly containing ammonium, sulfates and nitrates is the major part of the particulate matter. This is particularly true in the fine mode (D < 2.5 µm). The thermodynamic equilibrium model ISORROPIA [Nenes et al., 1998], is used to determine the particle/gas partitioning of semi-volatile inorganic species. The model calculate the thermodynamical equilibrium of the system: sulfate-nitrate-ammonium-sodium-chloride-water at a given temperature and relative humidity. The possible species are the following:

- **Gas phase**: NH₃, HNO₃, HCl, H₂O.
- **Liquid phase**: NH₄⁺, Na⁺, H⁺, Cl⁻, NO₃⁻, SO₄²⁻, HSO₄⁻, OH⁻, H₂O, HNO₃(aq), HCl(aq), NH₃(aq), H₂SO₄²⁻(aq), NH₄HSO₄, (NH₄)₂SO₄, NH₄Cl, NaCl, NaNO₃, NaHSO₄, Na₂SO₄.
- **Solid phase**: (NH₄)₂SO₄, NH₄HSO₄, (NH₄)₂H(SO₄)₂.

Due to its low vapor pressure, sulfuric acid is entirely transferred in the condensed phase. Also, the Sodium is located in the particulate phase. Inorganic aerosols can be a mix of solid and liquid species depending on temperature and humidity. The solid/liquid phase transition is solved by ISORROPIA by computing the deliquescent relative humidities (transition relative humidity between the phases). In the CHIMERE model, the calculation of the thermodynamical equilibrium can be done by interpolating a look-up table (see characteristics in Table 10.5). This look-up table has been pre-calculated and is delivered with the model in the file AEROMIN.bin. The partitioning coefficient for the nitrates and ammonium, and the aerosol water content has been calculated for a range of temperature from 260 to 312K, for relative humidity from 0.3 to 0.99 and for concentrations from 10⁻² to 65 µ.g.m⁻³. Because of numerical limits, Sodium and Chloride are not accounted for in this table. The active seassalt version needs the to use the on-line coupling.
<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
<th>Increment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature (K)</td>
<td>260</td>
<td>312</td>
</tr>
<tr>
<td>Relative Humidity</td>
<td>0.3</td>
<td>0.99</td>
</tr>
<tr>
<td>(\text{H}_2\text{SO}_4, \text{HNO}_3, \text{NH}_3) (\text{(\mu\text{g.m}^{-3})})</td>
<td>(10^{-2})</td>
<td>65</td>
</tr>
</tbody>
</table>

Table 10.5: Characteristics of the look-up table used for the calculation of the thermodynamic equilibrium with ISORROPIA.

The use of the look-up table allows to run the model faster, some errors can occur around each deliquescent point. This approach has been compared to the on-line coupling and tested on an entire year (2001) at the regional scale (0,5°x0,5°) over Europe.

Table 10.6: Relative humidity at deliquescent points for the species used by ISORROPIA in the system sulfate-nitrate-ammonium-water.

<table>
<thead>
<tr>
<th>Species</th>
<th>DRH (298.15K)</th>
<th>Mixing</th>
<th>MDRH (298.15K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>((\text{NH}_4)_2\text{SO}_4)</td>
<td>0.799</td>
<td>((\text{NH}_4\text{NO}_3, (\text{NH}_4)_2\text{SO}_4))</td>
<td>0.600</td>
</tr>
<tr>
<td>(\text{NH}_4\text{NO}_3)</td>
<td>0.618</td>
<td>((\text{NH}_4\text{HSO}_4, \text{NH}_4\text{SO}_4))</td>
<td>0.360</td>
</tr>
<tr>
<td>(\text{NH}_4\text{HSO}_4)</td>
<td>0.400</td>
<td>((\text{NH}_4\text{HSO}_4, (\text{NH}_4)_2\text{SO}_4))</td>
<td>0.675</td>
</tr>
<tr>
<td>((\text{NH}_4)_3\text{H(SO}_4)_2)</td>
<td>0.690</td>
<td>((\text{NH}_4)_3\text{H(SO}_4)_2, (\text{NH}_4)_2\text{SO}_4)</td>
<td>(0.1) to (2.8) (\mu\text{g.m}^{-3}).</td>
</tr>
</tbody>
</table>

The comparison shows the use of an on-line coupling leads to a weak decrease of the mean concentrations (13% for the nitrates, and no more than 2% for the sulfates) on the EMEP site. Ammonium concentrations are slightly increase (1 to 5%). In absolute values, the differences never exceed 0.5 \(\mu\text{g.m}^{-3}\) in average for the nitrates and 0.1 \(\mu\text{g.m}^{-3}\) for the sulfates and ammonium. The aerosol water content is slightly decreased (3 to 13% ; 0.1 to 2.8 \(\mu\text{g.m}^{-3}\)).

The sensitivity tests showed very weak differences, less than ± 20%. The differences are higher in winter compare to summer. The highest differences are observed above 50-60% for the nitrates and ammonium corresponding to the main deliquescent points. Indeed, the look-up table is not enough refined in this zone to account for the strong variations of the concentrations. For the water, the highest differences are observed in the range 95-100% where the absorption of water can increase by a factor of 1000. The differences do not depend on the temperature (not shown here).

The differences obtained when comparing the on-line coupling and the look-up table are small enough compare to the uncertainties in the modelling of the other processes. The look-up table of ISORROPIA is able to determine the partition of NH\(_4\)/NH\(_3\) and HNO\(_3\)/NO\(_3\).

10.3.7 Multiphase chemistry

10.3.7.1 Sulfur aqueous chemistry

If the aerosol option of the model is selected, Aqueous sulphate chemistry is considered; Sulfate is produced in the following aqueous reactions ([Berge, 1993]; [Hoffmann and Calvert, 1985]; [Lee and Schwartz, 1983]):

- \(\text{SO}_2^{aq} + O_3^{aq} \rightarrow \text{SO}_4^{2-}\)
- \(\text{HSO}_4^{-} + O_3^{aq} \rightarrow \text{SO}_4^{2-}\)
- \(\text{SO}_2^{2-} + O_3^{aq} \rightarrow \text{SO}_4^{2-}\)
- \(\text{SO}_2^{2-} + \text{H}_2\text{O}_2^{aq} \rightarrow \text{SO}_4^{2-}\)
- \(\text{SO}_2^{aq} + \text{NO}_2^{aq} \rightarrow \text{SO}_4^{2-}\)
- \(\text{SO}_3^{2-}(\text{Fe}^{3+}) \rightarrow \text{SO}_4^{2-}\)
\( \text{HSO}^-_{3}(Mn^{2+}) \rightarrow \text{SO}^{2-}_{4} \)

SO\(_2\), H\(_2\)O\(_2\) and O\(_3\) in the aqueous phase are in equilibrium with the concentrations in the gas phase. Moreover, aqueous SO\(_2\) is dissociated into HSO\(_{-}^{3}\) and SO\(_{3}^{-2}\). Catalyzed oxidation reactions of sulfur dioxide in aqueous droplets with iron and manganese are considered, following [Hoffmann and Calvert, 1985] among others. Henry’s law coefficient and other aqueous equilibrium constants are used ([Seinfeld and Pandis, 1998]). Sulfur chemistry is very pH sensitive. pH is kept bound between 4.5 and 6.0.

### 10.3.7.2 Heterogeneous chemistry

Again with the aerosol option of the model, a few heterogeneous reactions are also considered. Nitric acid is produced onto existing particles and fog droplets. Although aerosol particles and cloud droplets occupy a very small fraction of the atmosphere, it is now well established that reactions involving gas species onto their surfaces may significantly contribute to atmospheric chemistry cycles. [Jacob, 2000] recommends for ozone model to include a minimal set of reactions with associated uptake coefficients given by [Harrison and Kito, 1990], and other references in [Jacob, 2000]:

- \( \text{HO}_2 \rightarrow 0.5\text{H}_2\text{O}_2 \) \( \gamma = 0.2 \)
- \( \text{NO}_3 \rightarrow \text{HNO}_3 \) \( \gamma = 0.001 \)
- \( \text{NO}_2 \rightarrow 0.5\text{HNO}_3 + 0.5\text{HONO} \) \( \gamma = 0.0001 \)
- \( \text{N}_2\text{O}_5 \rightarrow 2\text{HNO}_3 \) \( \gamma = 0.01 - 1 \)

The first-order rate constant \( k \) for gas heterogeneous loss onto particles is given by:

\[ k = \sum_l \left( \frac{d_l}{2D_g} + \frac{4}{V\gamma} \right)^{-1} A_l \]

(10.13)

with \( d_l \), the particle diameter (m), \( D_g \), the reacting gas molecular diffusivity (m\(^2\)s\(^{-1}\)), \( n \), the mean molecular velocity (m s\(^{-1}\)), \( A_l \), the total surface area in the particle bin \( l \) and \( \gamma \) the uptake coefficient of reactive species. The uptake coefficient for N\(_2\)O\(_5\) is assumed to be temperature-dependent in the range 0.01 - 1 ([De Moore et al., 1994]) with increasing values for decreasing temperatures. A recent study ([Aumont et al., 2003]) suggests that NO\(_2\) reactions on wet surfaces could be an important source for HONO production during wintertime smog episodes, so, a new reaction is added (also present in the gas-phase mechanism, see above).

### 10.3.8 Secondary organic aerosol chemistry

The complete chemical scheme implemented in CHIMERE includes biogenic and anthropogenic precursors ([Table 10.7]). Biogenic precursors include API (\( \alpha \)-pinene and sabinene), BPI (\( \beta \)-pinene and \( \delta \)-3-carene), LIM (limonene), OCI (myrcene and ocimene) and ISO (isoprene). Anthropogenic precursors include TOL (benzene, toluene and other mono-substituted aromatics), TMB (Trimethylbenzene and other poly-substituted aromatics), and NC4H10 (higher alkanes). SOA formation is represented according to a single-step oxidation of the relevant precursors and gas-particle partitioning of the condensable oxidation products. The gas-particle partitioning formulation has been described in detail by [Pun et al., 2006]. The overall approach consists in differentiating between hydrophilic SOA that are most likely to dissolve into aqueous inorganic particles and hydrophobic SOA that are most likely to absorb into organic particles. The dissolution of hydrophilic SOA is governed by Henry’s law whereas the absorption of hydrophobic particles is governed by Raoult’s law. The large number of condensable organic compounds is represented by a set of surrogate compounds that cover the range of physico-chemical properties relevant for aerosol formation, i.e., water solubility and acid dissociation for hydrophilic compounds and saturation vapor pressure for hydrophobic compounds. These surrogate compounds were selected by grouping identified particulate-phase molecular products with similar properties. The molecular weight of each surrogate compound is determined based on its structure and functional
The Henry’s law constant or the saturation vapor pressure of the surrogate species is derived from the average properties of the group. Other properties are estimated using the structure of each surrogate compound. Enthalpy of vaporization are given in brackets (kJ.mol\(^{-1}\)) for each SOA compounds: AnA0D (88), AnA1D(88), AnA2D(88), BiA0D(88), BiA1D(88), BiA2D(109), AnBmP(88), AnBmP(88), BiBmP(175). The full name of compounds are explicited in Table 10.7 caption. The absorption process in CHIMERE is implemented as in [Bowman et al., 1997]. A dynamical approach is adopted to describe the gas/particle conversion since the model time-step is about 5 min. and using the approach by [Bowman et al., 1997], the characteristic time for mass transfer can exceed 20 min. for coarse particles.

\[
J_i = \frac{1}{\tau_i} (G_i - G_i^{eq})
\]  

(10.14)

\(J_i\) (\(\mu g.m^{-3}.s^{-1}\)) is the absorption or desorption flux of species \(i\), \(\tau_i\) (s) is a characteristic time of the mass transfer that depends on particle size and the chemical properties of species \(i\), \(G_i\) is the bulk gas-phase concentration of species \(i\) and \(G_i^{eq}\) is the gas-phase concentration of species \(i\) at thermodynamic equilibrium (i.e., at the surface of the particle). The equilibrium gas-phase concentrations are functions of the particle chemical composition, temperature and, for hydrophilic species, relative humidity, as described by [Pun et al., 2006]. The base SOA module was tested against the smog chamber data of [Odum et al., 1997] for anthropogenic compounds and those of [Griffin et al., 1999] for biogenic compounds and was shown to satisfactorily reproduce SOA formation for those compounds [Pun et al., 2006]. Higher alkanes and isoprene were added to the original chemical mechanism of [Pun et al., 2006]. The formation of SOA from higher alkanes follows the formulation of [Zhang et al., 2007] for the stoichiometric SOA yield and it is assumed that the SOA species can be represented by a hydrophobic surrogate compound with a moderate saturation vapor pressure. The formation of SOA from the oxidation of isoprene by hydroxyl radicals is represented with two surrogate products and follows the formulation of [Kroll et al., 2006, Zhang et al., 2007].

### 10.4 Impact of clouds

#### 10.4.1 Impact on photolysis

In this version clouds are assumed to lie above the model top, so that there is no cloud albedo effect within the model domain depth. For all photolysed species, clear sky photolysis rates \(J_c(z)\) are multiplied throughout model columns by an attenuation coefficient \(A(d)\) depending on the total cloud optical depth (COD) \(d\). Using the TUV model, and a large set of CODs for clouds at various altitudes, the attenuation relative to the clear-sky case has been fitted as a function of COD with the formula:

\[
A(d) = e^{-0.11d^{2/3}}
\]  

(10.15)

Several options are offered in order to calculate the COD. Total COD, \(d\), is the sum of partial CODs from 3 cloud layers, low clouds \(d_l\), medium clouds \(d_m\) and high clouds \(d_h\). The limits between these cloud is user-chosen, but depend on the meteorological model. For MM5, limits of 2000m and 6000m are proposed. For each cloud layer three options are possible for the calculation of the partial cloud optical depth:

- Calculation as a function of Liquid/Ice Water Content in the column; using an assumption of sphericity and equivalent droplet size of 6 microns, an assumption of hexagonal shape for ice particles, the formula for cloud optical depth is \(180.C_w + 67.C_i\), where \(C_w\) and \(C_i\) are respectively the liquid water column (in Kg/m\(^2\)) and ice column for this cloud layer.
- Liquid/Ice water are generally unverified and unstable parameters in atmospheric models. Basing a cloud parameterization on such parameters can be risky. A more robust parameterization consists in using relative humidity only. The proposed parameterization consists in parameterizing the COD as a function of the integral \(R\), over the cloud depth, of the relative humidity above 75%. It is assumed that small cloud formation (in particular cumulus clouds) starts at 75% relative humidity. Normalization of
Reactions | kinetic rates ($\text{molec.cm}^{-3}\cdot\text{s}^{-1}$)
--- | ---
TOL+OH $\rightarrow 0.004 \times \text{AnA0D} + 0.001 \times \text{AnA1D} + 0.084 \times \text{AnBmP} + 0.013 \times \text{AnBIP}$ | $1.81 \times 10^{-12}\exp(355/T)$
TMB+OH $\rightarrow 0.002 \times \text{AnA0D} + 0.002 \times \text{AnA1D} + 0.001 \times \text{AnA2D} + 0.088 \times \text{AnBmP} + 0.006 \times \text{AnBIP}$ | $9.80 \times 10^{-9}/T$
NC4H10+OH $\rightarrow 0.07 \times \text{BiA0D} + 1.36 \times 10^{-12}\exp(190/T)$
API+OH $\rightarrow 0.30 \times \text{BiA0D} + 0.17 \times \text{BiA1D} + 0.10 \times \text{BiA2D}$ | $1.21 \times 10^{-11}\exp(444/T)$
API+NO3 $\rightarrow 0.80 \times \text{BiBmP}$ | $1.01 \times 10^{-15}\exp(-732/T)$
BPI+OH $\rightarrow 0.07 \times \text{BiA0D} + 0.08 \times \text{BiA1D} + 0.06 \times \text{BiA2D}$ | $2.38 \times 10^{-11}\exp(357/T)$
BPI+O3 $\rightarrow 0.09 \times \text{BiA0D} + 0.13 \times \text{BiA1D} + 0.04 \times \text{BiA2D}$ | $1.50 \times 10^{-17}$
LIM+OH $\rightarrow 0.20 \times \text{BiA0D} + 0.25 \times \text{BiA1D} + 0.005 \times \text{BiA2D}$ | $2.51 \times 10^{-12}$
LIM+O3 $\rightarrow 0.09 \times \text{BiA0D} + 0.10 \times \text{BiA1D}$ | $1.71 \times 10^{-10}$
OCI+OH $\rightarrow 0.70 \times \text{BiA0D} + 0.075 \times \text{BiA1D}$ | $2 \times 10^{-16}$
OCI+O3 $\rightarrow 0.50 \times \text{BiA0D} + 0.055 \times \text{BiA1D}$ | $5.10 \times 8/T$
OCI+NO3 $\rightarrow 0.70 \times \text{BiA0D} + 0.075 \times \text{BiA1D}$ | $7.50 \times 10^{-14}/T$
ISO+OH $\rightarrow 0.232 \times \text{ISOPA1} + 0.0288 \times \text{ISOPA2}$ | $4.30 \times 10^{-9}/T$

Table 10.7: *Gas phase chemical scheme for SOA formation in CHIMERE.* The surrogate SOA compounds consist of six hydrophilic species that include an anthropogenic nondissociative species (AnA0D), an anthropogenic once-dissociative species (AnA1D), an anthropogenic twice-dissociative species (AnA2D), a biogenic nondissociative species (BiA0D), a biogenic once-dissociative species (BiA1D) and a biogenic twice-dissociative species (BiA2D), three hydrophobic species that include an anthropogenic species with moderate saturation vapor pressure (AnBmP), an anthropogenic species with low saturation vapor pressure (AnBIP) and a biogenic species with moderate saturation vapor pressure (BiBmP), and two surrogate compounds for the isoprene oxidation products.

$\mathbf{R}$ leads to the formulation (for instance for low clouds): $d_{l} = a\mathbf{R}/dz$, where $a=0.02$ is chosen such that a 1000m-thick layer has an optical cloud depth of 20.

- An even simpler parameterization can be achieved by making the COD simply proportional to the cloud fraction (if available) for each cloud layer. Coefficient tuning led to proportionality coefficients of: 50 for low-clouds, 10 for medium clouds and 2 for high clouds. This means, for instance, that a sky covered with 100% of high clouds has an optical depth of 2. Tuning was performed with ECMWF cloud fraction data and should change with the meteorological model.

**Recommendations** The first option using liquid/ice water (whenever available), is based on a variable which can be very model-dependent and which is rarely verified against observations. Moreover it does not take into account fractionary cloudiness. However it may be suited for high/medium clouds which are often stratiform clouds in the midlatitudes. The second option uses cloud fractions (whenever available), which is less meaningful to radiation but could be used when cloud/ice water is not available. The third option uses relative (to liquid water) humidity, and has been tuned using J(NO2) measurements taken over a long period near Paris (manuscript in preparation). The formulation, modifying radiation for RH $> 0.75$ should only be used for low clouds. It has the advantage of being a more robust parameterization since it depends on a highly verified variable. In summary, our preference is: RH formulation for low clouds, and for liquid/ice water formulation (whenever available) for medium and high clouds, and cloud fractions otherwise.

The attenuation coefficient is calculated in the `src/diag/diagmet.f90` diagnostic interface model. It is read in `src/initio/iniphys.f90`, photolysis rates are calculated in routine `src/model/photorates.f90` every coarse time step.
10.4.2 Wet scavenging

10.4.2.1 In cloud scavenging

In cloud, particle scavenging is difficult to model. Particles can be scavenged either by coagulation with cloud droplets or by precipitating drops. Particles also act as cloud condensation nuclei to form new droplets. This latter process of nucleation is the most efficient one in clouds. According to [Tsyro, 2002] and [Guelle et al., 1998], the deposition flux is written as:

\[
\frac{dQ_{kl}}{dt}_{incl} = \frac{\zeta_1 p_r}{w_la}Q_{kl}^k
\]

(10.16)

with \(p_r\) is the precipitation rate released in the grid cell (g cm\(^{-2}\) s\(^{-1}\)), \(w_l\) the liquid water content (g cm\(^{-3}\)), \(h\) the grid height (cm) and \(\zeta\) an empirical uptake coefficient (in the range 0-1) depending on particle composition.

10.4.2.2 Sub-cloud scavenging

Particles are scavenged by raining drops, the deposition flux of particles being given by:

\[
\frac{dQ_{kl}}{dt}_{subcl} = -\frac{apE}{u_g}Q_{kl}^k
\]

(10.17)

with \(a\) is an empirical coefficient, \(p\) the precipitation rate in the grid cell (g cm\(^{-2}\) s\(^{-1}\)), \(E\) a collision efficiency coefficient between particles and raining drops ([Slinn, 1983] and \(u_g\) the falling drop velocity (cm s\(^{-1}\)). Assuming a constant drop diameter (2 mm), this parameterization is an approximation of equations described in [Seinfeld and Pandis, 1998] and [Jung et al., 2002]. In the next developments, this equation will be improved.

10.5 Radiative transfers and photochemical reaction rates

10.5.1 Processes taken into account

Up to version 2013b, CHIMERE worked exclusively with tabulated photochemical reaction rates, precalculated using the TUV model, and using a simple parameterization for attenuation by clouds. The photolysis rates were therefore assumed constant on the vertical, and depended only on the zenithal angle and on the presence of clouds, which were assumed to be over model top. These assumptions were justified by the fact that CHIMERE was historically a boundary-layer model.

Since version 2014a, CHIMERE can take into account the following effects on photolysis:

- Effect of ice- and liquid-water clouds on photolysis rates through Mie diffusion
- Effect of aerosols on photolysis rates through absorption and Mie diffusion
- Effect of absorption by ozone on photolysis rates, using real-time ozone concentrations within the model domain instead of climatologies

This has been obtained by including the Fast-JX model for radiative transfer (version 7.0b, see [Wild et al., 2000, Bian et al., 2002]) inside CHIMERE. This model is a model for radiative transfer and photochemical rates that has been designed with the purpose of its inclusions in CTMLs, and is already used in models such as Polair3D, Geos-Chem, UKCA and PHOTOMCAT (e.g. [Voulgarakis et al., 2009, Real and Sartelet, 2011, Telford et al., 2013]). The photolysis rates calculated by fast-JX have been validated in the boundary layer ([Barnars et al., 2004]) as well as in the free troposphere ([Voulgarakis et al., 2009]). Fast-JX is designed to reduce as much as possible the computational cost as much as possible without inducing errors of more than 5% on photochemical reaction rates. Actually, in CHIMERE, the additional computation cost compared to the former formulation with tabulated rates is below 10% of the total computation cost.
From a computational point of view, the calculation of photochemical reaction rates is performed in three steps (Fig. 10.2):

1. Preprocessing of aerosol optical properties (Mie scattering and absorption) for each aerosol species and bin, generate input files for Fast-JX: necessary only when changing aerosol species or their optical properties
2. Initialisation of Fast-JX model (read input files): at the beginning of each run
3. Online calculation of photochemical reaction rates (every physical time step)

Figure 10.2: Routines, files and scripts involved in the calculation of radiative transfers

10.5.2 Optical preprocessing using prep_mie

The Mie calculations for each aerosol species and bins is performed by a short standalone program named prep_mie.F90 (in the src/prep directory). This program is called by chimere-step1.sh and runs in the temporary execution directory. The name of its input and output files is stored in the prep_mie.nml file, in the same directory. prep_mie.F90 needs three input files:

1. AEROSOL: number of bins, their diameters and the list of the AEROSOL species,
2. input-fastj.txt: optical properties of each aerosol species (real and imaginary part of the refraction indices for 5 wavelength - 200 nm, 300 nm, 400 nm, 600 nm and 999 nm), as well as the density and Hanel size growth coefficient. This file needs to include these quantities for ALL aerosol species listed in the AEROSOL file. If the user adds a new aerosol species, he will need to put its optical and physical properties in the input-fastj.txt file by editing it manually. Species in input-fastj.txt do not need to be in the same order as in the AEROSOL file, but it is requested that all aerosol species listed in the AEROSOL file shall be present in the input-fastj.txt file, with exactly the same name.
3. ACTIVE_SPECIES: list of the active species. This file is used only to check whether prep_mie writes its outputs with all the aerosol species in the right order.
It is worth noting that Fast-JX (as well as CHIMERE) treats distinct bins of a given aerosol species as distinct species. Therefore, prep_mie will perform the Mie calculations for $n_{bins} \times n_{aerospec}$ species. The output file of prep_mie is stored in FJX_scat-aer.dat. This file includes, for each of the $n_{bins} \times n_{aerospec}$ species, the effective radius, density, the efficiency factor $Q$, the single-scattering albedo and the first 7 terms of the Taylor expansion of the scattering phase function. These values are written in the exact same order as the order of the aerosol species in the ACTIVE_SPECIES file.

The Mie calculation is based on Michael Mischenko’s spher.f code (which is distributed with CHIMERE as well). As it is a relatively long calculation (up to a couple of minutes depending on the computer and on the number of aerosol species and bins), it is performed only if the FJX_scat-aer.dat is absent in the inputdata directory. Therefore, if the user modifies the optical or physical properties of the aerosols in input-fastj.txt, he will need to remove the FJX_scat-aer.dat file from the inputdata directory in order to force recalculation of the scattering phase functions.

10.5.3 Fast-JX initialisation

Fast-JX initialisation is performed by the inifastj.F90 routine. This routine is a wrapper for the INIT_FJX routine of the module fjx_init_mod.f90. INIT_FJX reads the following input files:

1. FJX_spec.dat: cross-sections for photochemical reaction rates.
2. FJX_scat-cld.dat: cloud scattering data
3. FJX_scat-UMa.dat: University of Michigan aerosol scattering data (not used)
4. atmos_std.dat: temperature and ozone climatology - used for radiative transfers above the simulation domain
5. FJX_j2j.dat: file containing the information needed to reorder Fast-JX photochemical reaction rates in the order needed by the CTM - in this case, CHIMERE.

The values read from these input files are stored in arrays that are used for the online calculation of photochemical reaction rates at each physical time step.

10.5.4 Online calculation of photochemical reaction rates

The calculation of the photochemical reaction rates is performed by routine photorates_fastj.F90, which calls the fast-jx PHOTO_JX routine (in fjx_sub_mod.f90) for each atmospheric column, after filling the input arrays of Fast-JX with the values from the meteorological model (for clouds) and from CHIMERE (for ozone and aerosols). photorates_fastj.F90 finally takes into account the clouds above model top by a simple calculation of the attenuation factor - whereas clouds within the CHIMERE domain are taken into account in details, separating water- and ice-clouds and performing an explicit Mie calculation.

10.5.5 Using the old photorates?

In CHIMERE versions 2014, it is still possible to use the tabulated photolytic rates from TUV, just as in previous version. To use this option, the switch $ifastj$ in chimere.par needs to be set to 0. However, this option will become deprecated in the next distributed version of CHIMERE, and we strongly encourage all users to use the new scheme for radiative transfers.
Bibliography


Appendix A

References using CHIMERE

A.1 Reference papers

For CHIMERE description overview: see [Menut et al., 2013, GMD]
http://www.geosci-model-dev.net/6/981/2013/gmd-6-981-2013.html


For CHIMERE used in real-time forecast: see [Rouil et al., 2009] or [Menut and Bessagnet, 2010]


For CHIMERE used for health impacts: see [Valari et al., 2010]

- Valari M. and L.Menut, 2010, Transferring the heterogeneity of surface emissions to variability in pollutant concentrations over urban areas through a chemistry transport model, Atmospheric Environment, Volume 44, Issue 27, Pages 3229-3238

For CHIMERE used for fires emissions: see [Turquety et al., 2014, GMD]


For CHIMERE used for dust: see [Menut et al., 2013, JGR]


A.2 List of papers


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Appendix B

History

This section tracks the model evolution over the last versions.

B.1 chimere2008

Version chimere2008 contained the following improvements and new processes.

- New functionality:
  - Due to integration of the MEGAN model biogenic emission potentials data and emission rates parameterizations, Chimere can now be used outside Europe if the user provides anthropogenic emissions in the region of interest
  - Automatic preparation of the file `LANDUSE_<domain>` from the original GLCF global land use database for the desired Chimere domain
  - Meteorological interface to the WRF model prepwrf has been added
  - Possibility to use aerosol boundary and initial conditions from the LMDz model output
  - A new mode of exachim to display various data slices by a simple mouse click

- Process changes:
  - Updated Secondary Organic Aerosols (SOA) chemistry: the full MEGAN SOA scheme is now used

- Computational changes:
  - New format of the emissions interface emiSURF and prepemis. The emission files are now separated by individual species, which makes the prepemis interface simpler and easier to modify. If a simulation spans two consequent months, emissions for each day are now taken from a corresponding month rather than from the first month for all days. One can also choose emission types to use independently: either surface, point, or fire emissions. Hourly changes of fire emissions are now allowed. If emissions are not available for a given species, they are set to zero, and the simulation continues
  - Reorganized boundary and initial conditions interface for more convenience and code simplicity. User can now choose a global database for each species
  - Revised vertical interpolations in the boundary and initial conditions interface
  - Running Open MPI or LAM depending on user system settings. If both realizations are found, preference is given to Open MPI
  - Simulation parameters are now organized in the form of an array in the top calling script chimere.sh. This allows more convenient parameter specification, especially for simulations for several, possibly nested, model domains
  - The script chimere-run.sh has been split into parts corresponding to Chimere components: compilation, meteorological interfaces, emissions, initial and boundary conditions, and Chimere core. It is now possible to run individually one or more of these components.
B.2 V200606

B.2.1 Parallelization

Version V200606 represented a major breakthrough in the model computational speed, since it has been parallelized and can now run on distributed memory clusters and shared memory machines, ranging from the local home-made cluster of PCs, to large supercomputers. However, there are no changes neither in the scientific core of the model, nor in the I/O file formats.

The rationale of the parallelization was:

- the increasing computation time of the aerosol version and of nextcoming, more sophisticated versions,
- the user requirements for higher resolution domains,
- the requirements of air pollution forecast agencies, in terms of forecast computation time.

CHIMERE uses the distributed memory scheme, and an MPI message passing library. It has been tested with Open MPI and LAM/MPI, but should work, with minor changes in the scripts, with MPICH or other MPI compatible parallel environments.

There is one master program, which calls several worker subroutines, each worker been in charge of the processing of a subdomain. Subdomains are the result of a Cartesian division of the main geographical domain by the number of processors.

The master program is in charge of the initializations and file I/O. The workers are in charge of the scientific processing and inter-subdomains boundary conditions updates.

As described above, CHIMERE is basically an MPMD (multiple program, multiple data) application. However, MPMD is only available with MPI-2 compatible environments. To increase CHIMERE portability, its interface has been tweaked to mimic the appearance of an SPMD (single program, multiple data) application, which makes it compatible with widely spread MPI-1 parallel environments.

Despite the tremendous architectural change in the code structure, most scientific subroutines, now called by the worker main subroutine, have remained unchanged.

As far as the user interface is concerned, the only apparent modifications are:

- definition of subdomains in chimere-mm5 script: nzdoms and nmdoms parameters.
- use of an MPI library: MPI must be installed for running CHIMERE, even if it runs on only one processor with only one subdomain.

B.2.2 Toolbox

There is a new processing inside exachim: the COARDS intermediate file is no longer necessary. Instead, GrADS compliant files are built directly. A new utility, chm2grads.f90, replaces chm2coards.f90. All kinds of CHIMERE grids may be used, not only rectilinear ones. More sophisticated command line options allows for displaying only selected variables and time slots.

The udunits library is no longer used.

A new tool to transform the old CHIMERE binary files into netCDF files, chmbin2cdf.f90, has been included in the distribution.

An older tool, chim2fig, which used to be distributed with pre-netCDF versions of CHIMERE, has been upgraded to accept netCDF files.

B.2.3 Scripts

New top-level scripts have been added, to run CHIMERE on PC clusters with a PBS-like batch scheduler. Despite the fact that an interface to ECMWF meteorology is not yet provided in this version, a script to run CHIMERE on ECMWF HPCD computer is provided as an example for running CHIMERE under IBM LoadLeveler and POE environments.
B.2.4 makefiles changes

The directory structure of the src/ tree has been modified, and Makefiles have been rationalized. This allows now for using the parallel compilation capability of the GNU make utility. Also, the meteo interface is run in background, during model compilation. This reduces dramatically the compilation time on multiprocessor machines, allowing for more sophisticated optimizations. Minor bugs have been corrected in Makefile headers.
Appendix C

Some scripts used in the CHIMERE suite

C.1 The `domains/makeCOORDdomains` script for horizontal grid definition

To create a new COORD file, you first have to add a new line in the `domainlist.nml` file describing your new domain. After that, run manually the `makeCOORDdomains` script (in the `domains/` directory or here below) with the required domain name:

```
makeCOORDdomains CONT3
```

with the following `makeCOORDdomains` script:

```
#!/bin/sh
if [ $# -eq 0 ] ; then
  echo "define the domain name"
  exit 0
else
  dom=$1
fi

nzo='gawk '$1=="${dom}" {print $2}' domainlist.nml'
name='gawk '$1=="${dom}" {print $3}' domainlist.nml'
dx='gawk '$1=="${dom}" {print $4}' domainlist.nml'
dy='gawk '$1=="${dom}" {print $5}' domainlist.nml'
xbotleft='gawk '$1=="${dom}" {print $6}' domainlist.nml'
ybotleft='gawk '$1=="${dom}" {print $7}' domainlist.nml'

touch COORD
rm COORD
[[ -z ${nzo} || -z ${name} || -z ${dx} || -z ${dy} || -z ${xbotleft} || -z ${ybotleft} ]] &&
  { echo "Error reading domainlist.nml. Probably domain ${dom} is not defined. Bye" ; exit 1 ; }

echo " making horizontal COORD file"
echo " geometry definition:"
echo " nodes="${nzo}"x"${name}"
echo " resol="${dx}"x"${dy}"
echo " south-west point="${xbotleft}"x"${ybotleft}"

gawk -v xbotleft=${xbotleft} -v ybotleft=${ybotleft} -v dx=${dx} -v dy=${dy} -v nzo=${nzo} -v nme=${name} -v dom=${dom} -v domindex=${domindex} -v syst=${syst} -- 'BEGIN{
  for(j=1;j<=nme;j++){
    for(i=1;i<=nzo;i++){
      x=(i-1)*dx
      y=(j-1)*dy
      xlon=xbotleft+x
      xlat=ybotleft+y
    }
  }
}'
```

C.2 The *util/define_geom* script for vertical grid definition

To make your own VCOORD file, go to the directory *util/*, edit the *define_geom* script and adapt the top pressure level to the one you need.

**N.B.:** It is recommended to have a maximum ptop of 200 hPa since the global model used for boundary conditions delivered data only up to this value.

*The define_geom script:*

```bash
#!/bin/sh

# Defines a geometrical-progression vertical layering
# For the CHIMERE model. It actually produces sets of
# Hybrid sigma-p coefficients Ak and Bk such that the
# pressure at top of layer k is Pk = Ak*1e5 + Bk*Ps in Pa
# where Ps is Surface pressure

# Define the parameters below and run the script by just typing "define_geom"

ptop=700   # Pressure at model top
nlay=8     # Number of layers
pre1=995   # Pressure (hPa) of the first layer top when Ps = 1000 hPa
fout=../data/vgrid/VCOORD.8GEOM700

echo ${nlay} ${pre1} ${ptop} | gawk -f geom.awk > ${fout}
```

**Recommendations**

- When defining manually the hybrid coefficients the user shall verify that under all possible meteorological conditions these layers do not cross one another or get mixed up.
- It is highly recommended that top level be a pressure level (b_k = 0), since it has been found to minimize mass loss through top boundary.
- Using the MOZART and LMDz-INCA boundary conditions, one should not use a model top above 200 hPa.
- In the present formulation for cloud/radiation/photolysis, it is assumed that the model domain is *below the clouds*, i.e. no cloud albedo is taken into account. This puts constraints on model top to be not too high. This will be changed in future releases.
Appendix D

How To install NetCDF under GNU/Linux

D.1 Background

Since CHIMERE requires a NetCDF package. This note describes how to install NetCDF for the supported compilers.

NetCDF installation has been tested with:

- ifort 32 bits (version 8.1.028)
- ifort 64 bits (version 8.1.027)
- g95 32 bits (version 0.92 20090624)
- g95 64 bits (version 0.91 20080227)
- gfortran 32 bits (version 4.4.2 20091027)
- gfortran 64 bits (version 4.1.2 20080704)
- pgf90 32 bits (version 5.2.4)
- pgf90 64 bits (version pgf90 6.0-5)
- netcdf (version 3.6.3 or 4.1.1 with hdf5-1.8.5)

D.2 Download

- Download NetCDF (source package) from the URL:
  cd /tmp
  wget ftp://ftp.unidata.ucar.edu/pub/netcdf/netcdf.tar.gz

- Decompress and detar
  tar xvzf netcdf.tar.gz

D.3 Configure NetCDF

At the time of writing of this How-To, the current version of NetCDF is 3.6.4. If you downloaded a newer version, replace 3.6.4 by the new version number in the following text.

    cd netcdf-3.6.3/src

The configuration process depends on several environment variables that you shall set according to your compiler. Although it may be possible to link CHIMERE executables compiled with compiler A with the NetCDF library compiled with compiler B, we strongly recommend to use the same compiler. The time you
will spend to install a new NetCDF library is negligible compared to the time you could lose trying to match inconsistent libraries.

We suppose you want to install netcdf somewhere under /opt. If you choose to install under /usr/local, or under your home directory, replace /opt your installation path in the following text.

We also suppose your shell is like bash or ksh. If you use csh, modify the export statements according to your shell syntax.

D.3.1 ifort

As root:

    mkdir /opt/netcdf-3.6.3-ifort

As an ordinary user:

    export FC=ifort
    export F90=ifort
    export FFLAGS="-fltconsistency"
    export CPPFLAGS="-DNDEBUG -DpgiFortran"
    ./configure --prefix=/opt/netcdf-3.6.3-ifort
    make
    make test

    As root:

    make install

D.3.2 g95

As root:

    mkdir /opt/netcdf-3.6.3-g95

As an ordinary user:

    export CC='gcc'
    export CXX='g++'
    export CPPFLAGS=''-DNDEBUG -DgFortran'
    export CFLAGS=''-O -g'
    export FC='g95'
    export F77='g95'
    export FFLAGS=''-O -g -fno-second-underscore'""'
    export FCFLAGS=''-O -g -fno-second-underscore'"
    ./configure --prefix=/opt/netcdf-3.6.3-g95
    make
    make test

    As root:

    make install
D.3.3 pgf90

Some versions of pgf90 prior to 5.2 have experienced problems with the F90 interface of NetCDF. Do not try to install a library for which "make test" has failed.

As root:

```
mkdir /opt/netcdf-3.6.3-pgf90
```

As an ordinary user:

```
export CC=/usr/bin/gcc
export CPPFLAGS=''-DNDEBUG -DpgiFortran'
export CFLAGS=-O
export FC=pgf90
export FFLAGS="-O -w"
export CXX=g++
./configure --prefix=/opt/netcdf-3.6.3-pgf90
make
test
```

As root:

```
make install
```

D.3.4 ifort 64 bit on Intel EMT64 or AMD Opteron

As root:

```
mkdir /opt/netcdf-3.6.3-ifort
```

As an ordinary user:

```
export FC=ifort
export F90=ifort
export CFLAGS="-O -m64"
export FFLAGS="-mp"
export CPPFLAGS=''-DNDEBUG -DpgiFortran'
./configure --prefix=/opt/netcdf-3.6.3-ifort
make
test
```

As root:

```
make install
```

D.3.5 g95 64 bit on Intel EMT64 or AMD Opteron

As root:

```
mkdir /opt/netcdf-3.6.3-g95-64
```

As an ordinary user:

```
export CC='gcc'
export CXX='g++'
export CPPFLAGS=''-DNDEBUG -DgFortran'
```
export CFLAGS='\-O -m64'
export FC='g95'
export F77='g95'
export FFLAGS='\-O -g -fno-second-underscore'
export FCFLAGS='\-O -g -fno-second-underscore'
./configure --prefix=/opt/netcdf-3.6.3-g95-64
make
make test

As root:

make install

D.3.6  pgf90 64 bit on Intel EMT64 or AMD Opteron
Do not try to install a library for which "make test" has failed.
As root:

`# make install`

As root:

`# mkdir /opt/netcdf-3.6.3-pgf90-64`

As an ordinary user:

export CC=/usr/bin/gcc
export CPPFLAGS='\-DNDEBUG -DpgiFortran'
export CFLAGS=\-O
export FC=pgf90
export F90=pgf90
export FFLAGS="\-O \-w"
export CXX=g++
./configure --prefix=/opt/netcdf-3.6.3-pgf90-64
make
make test

As root:

`# make install`

D.4  Manually Configure CHIMERE

Automatic configuration of CHIMERE using config.sh is described in §2.2, p. 17. Here we explain how to
configure the model manually.
In the directory makefiles.hdr/, you will find 9 files:

Makefile.hdr.g95-64-lam
Makefile.hdr.g95-64-ompi
Makefile.hdr.g95-1am
Makefile.hdr.g95-ompi
Makefile.hdr.gfortran-64-lam
Makefile.hdr.gfortran-64-ompi
Makefile.hdr.ifort-64-lam
Makefile.hdr.ifort-64-ompi
Makefile.hdr.ifort-ompi
After linking to `Makefile.hdr` the file corresponding to your compiler, MPI library, and system (32 or 64 bit), for instance:

```
ln -sf makefiles.hdr/Makefile.hdr.g95-64-ompi Makefile.hdr
```

modify the lines `my_netcdflib=` and `my_netcdfinc=` in the file `mychimere.sh` to point to your NetCDF directory. Modify also the PATHs to your HDF5 library given by variables `my_hdflib` and `my_hdfinc`. For instance:

```
export my_netcddfdir=/opt/netcdf-3.6.3-g95
```

If you are using NetCDF4/HDF5:

```
export my_hdfdir=/opt/hdf5-1.8.5-g95
```

Follow the comments in `Makefile.hdr.xxxx` for other options.
Appendix E

How To install MPI under GNU/Linux

E.1 Background

CHIMERE is now parallelized, using the distributed memory scheme, and requires an MPI compatible Message Passing Library to be installed and configured on the host or cluster it will run on. 

MPI is required even if CHIMERE is planned to run on a single processor machine!

Several free MPI libraries are available for download. MPICH and LAM/MPI are well known. The newer OpenMPI is claimed to be the continuation of LAM/MPI. CHIMERE has been tested with LAM/MPI and Open MPI. This HOW-TO describes briefly the installation and basic configuration process for LAM/MPI and Open MPI on a RedHat-like GNU-Linux distribution.

We recommend the precompiled package installation for RedHat-like distributions. However, some 64 bit Linux distributions have a precompiled LAM-MPI binary which is not compatible with other libraries. In that case, you will have to install the LAM-MPI package from source, as described at the end of the document.

Tested with:

- Fedora Core 4
- LAM-7.1.1

E.2 LAM/MPI Installation

RedHat-like distributions include a RPM for LAM/MPI. It is generally called "lam". Here is the installation process for a Fedora Core 4 system. You must have administrative privileges to perform it.

- If you use YUM as a package tool:
  
yum install lam

- If you use RPM:
  
  ◦ download lam-7.1.1-7.FC4.i386.rpm from your Fedora repository
  ◦ you may also want libaio-devel-0.3.104-2.i386.rpm
  ◦ install :
    
    rpm -Uvh libaio-devel-0.3.104-2.i386.rpm lam-7.1.1-7.FC4.i386.rpm

- Edit /etc/lambda/lambda-host.def to set the list of hosts you will include in your LAM cluster. For instance, for a cluster of 3 bi-processors, lambda-host.def would contain:
For a uniprocessor machine, lam-bhost.def would only contain:

localhost

• Instead of using the system wide lam-bhost.def, you can create and use your own hosts file, and boot LAM/MPI using this file. A file named "nodelist.example" is provided as a template in this distribution. Edit it according to your environment.

E.3 Testing

• type:
  lamboot
to boot your LAM/MPI environment using system-wide hosts list, or
  lamboot <my_host_list>
to boot your own host list defined in file <my_host_list>

• type:
  lamnodes
to verify that all nodes declared in the hosts file are up.

If case of insuccess, get LAM/MPI documentation from their web site.
Most problems occur because the user is not allowed to perform rsh or ssh connexions to the hosts listed in hostfile.
Check with your system administrator that you can ssh to the target hosts. If the hosts are connected to a private network, ask her/him to allow rsh on these hosts. The advantage of using rsh is that you can schedule unattended jobs using cron or at. Otherwise you need to change your ssh passphrase for an empty one, which can be a security issue.

E.4 Uniprocessor users

Parallelism is mainly useful for Air Pollution Forecast Agencies, or for scientists running long periods of reananalysis. For the users who just want to run CHIMERE as they were accustomated to, on a single processor machine, here is a simple summary of what they shall do with LAM/MPI:

• install LAM/MPI as described above
  yum install lam

• check that ssh is installed on your machine
  ssh localhost
Most modern Linux distributions come with ssh installed and configured.

- edit `/etc/lam/lam-bhost.def` to keep only the line
  
  `localhost`

- boot LAM/MPI
  
  `lamboot`

- Enjoy CHIMERE!

### E.5 Installation from source

Thanks to Gabriele Curci at aquila.infn.it

Some 64 bit Linux vendors have compiled the lam package with the "second-underscore" option. This leads to an incompatibility between lam and netcdf libraries. If you get error messages like this in your make.log file, you are probably in that case:

```
  twostep_mod.f90:(.text+0xbdb6): undefined reference to ‘mpi_irecv_’
  twostep_mod.f90:(.text+0xc2cb): undefined reference to ‘mpi_issend_’
  twostep_mod.f90:(.text+0xc33a): undefined reference to ‘mpi_irecv_’
  twostep_mod.f90:(.text+0xc7f0): undefined reference to ‘mpi_issend_’
```

To overcome this problem, you have to install LAM-MPI from source. Here is the process, copied from Gabriele’s message:

- login as root
- download LAM source, I installed latest version 7.1.2 (wget http://www.lam-mpi.org/download/files/lam-7.1.2.tar.bz2)
- unzip the source (tar jxvf lam-7.1.2.tar.bz2)
- cd lam-7.1.2
- `./configure "FC=g77 -fno-second-underscore" --prefix=/usr/local`
- make
- make install

### E.6 Open MPI installation

This section briefly explains how to install Open MPI with g95 and ifort compilers from sources. The sources can be downloaded from the Open MPI home page [http://www.open-mpi.org](http://www.open-mpi.org).

**With g95 on a 32 bit system**

```
export COMPILO=g95
./configure CC=gcc CXX=g++ F77=$COMPILO FC=$COMPILO \  
  --prefix=/opt/openmpi-1.2.5-$COMPILO \  
  --with-mpi-f90-size=medium
make all
make install
edit /etc/profile to set the PATH variable
edit /etc/ld.so.conf.d/openmpi.conf
ldconfig
```
With g95 on a 64 bit system

```bash
export COMPILO=g95
./configure CC=gcc CXX=g++ F77=$COMPILO FC=$COMPILO \
    CFLAGS=-m64 CXXFLAGS=-m64 FFLAGS=-m64 FCFLAGS=-m64 \ 
    --prefix=/opt/openmpi-1.2.5-$COMPILO \ 
    --with-mpi-f90-size=medium
make all
make install
```

`edit /etc/profile to set the PATH variable`

`edit /etc/ld.so.conf.d/openmpi.conf`

`ldconfig`

Build options with ifort for 64 and a 32 bit systems

For a 64 bit system:

```bash
export CC=gcc
export CXX=g++
export CFLAGS=' -O2 -m64'
export CXXFLAGS=' -O2 -m64'
export LDFLAGS=' -O2'
export FC=ifort
export FCFLAGS=' -O2 -m64'
export F77=ifort
export FFLAGS=' -O2 -m64'
./configure --prefix=/opt/openmpi-1.2.5-ifort-64 --with-mpi-f90-size=medium
```

For a 32 bit system you need to remove the -m64 flag from the options above.
Appendix F

Notes on using CHIMERE with LAM MPI

You need to make sure that LAM MPI is booted on your system, with the right number of processors. The command to use is:

```
lamnodes
```

The system should respond with a list of active nodes and the number of processors per node. The total number of declared processors should be superior or equal to `nzdoms*nndoms` (see p.41).

If it does not, boot your MPI environment. With LAM/MP1, to boot the default nodes list, type:

```
lamhalt
lamboot
```

A file named `nodelist.example` is provided here as a template if you want to boot different nodes. To use this file, first edit it according to your environment, taking care to declare at least `nzdoms*nndoms` processors. Once your `nodelist.example` file is edited, type:

```
nzdoms
nndoms
```

If you want to have an understanding of the impacts of the hostlist file (nodelist.example) read the recommendations in p.41

F.1 Specific case of single node environment

In the trivial case of a single node environment, the node list file, either `/etc/lam/lam-bhosts.def` or your own `nodelist.example` should contain only this single line:

```
localhost
```

And you should set `nzdoms=1` and `nndoms=1` in `chimere.sh`.

In the other trivial case of a single bi-processor node, the node list file, should contain only this single line:

```
localhost cpu=2
```

And you should set `nzdoms=2` and `nndoms=1` in `chimere.sh`. 

165
Appendix G

Structure of the CHIMERE netCDF files

G.1 EMIS.[domain].[MM].[SPEC].s.nc and EMIS.[domain].[MM].[SPEC].p.nc

netcdf EMIS.CONT5.05.NO2.s {
  dimensions:
  Time = 24 ;
  west_east = 79 ;
  south_north = 47 ;
  bottom_top = 7 ;
  type_day = 7 ;
  SpStrLen = 23 ;
  variables:
    float lon(south_north, west_east) ;
    lon:units = "degrees_east" ;
    lon:long_name = "Longitude" ;
    float lat(south_north, west_east) ;
    lat:units = "degrees_north" ;
    lat:long_name = "Latitude" ;
    float EMEP_levels(bottom_top) ;
    EMEP_levels:units = "meters" ;
    EMEP_levels:long_name = "Cut_off_heights_for_redistribution" ;
    float NO2(Time, type_day, bottom_top, south_north, west_east) ;
    NO2:units = "molecule/cm2/s" ;
    NO2:long_name = "NO2 Emission" ;
  // global attributes:
  :Title = "CHIMERE emissions" ;
  :Sub-title = "Hourly surfacic emission" ;
  :Chimere_type = "EMISSIONS" ;
  :Generating_process = "Generated by sectoremis" ;
  :Conventions = "None" ;
  :Domain = "CONT5" ;
  :Year = "2003" ;
  :Landuse_for_Reggriding = "glcf" ;
  :history = "" ;
}

netcdf EMIS.CONT5.01.NO2.p {
  dimensions:
  Time = 24 ;
  west_east = 79 ;
  south_north = 47 ;
  Sources = 8 ;
  type_day = 3 ;
  variables:
float lon(south_north, west_east) ;
lon:units = "degrees_east" ;
lon:long_name = "Longitude" ;
float lat(south_north, west_east) ;
lat:units = "degrees_north" ;
lat:long_name = "Latitude" ;
long Sources_PIG(Sources) ;
Sources_PIG:units = "flag-0-1" ;
Sources_PIG:long_name = "Pig_treatment" ;
float Sources_lat(Sources) ;
Sources_lat:units = "Degrees" ;
Sources_lat:long_name = "Y_coordinate_of_source_point" ;
long Sources_ilat(Sources) ;
Sources_ilat:units = "cell_number" ;
Sources_ilat:long_name = "Y_coordinate_of_source_point" ;
float Sources_lon(Sources) ;
Sources_lon:units = "Degrees" ;
Sources_lon:long_name = "X_coordinate_of_source_point" ;
long Sources_ilon(Sources) ;
Sources_ilon:units = "cell_number" ;
Sources_ilon:long_name = "X_coordinate_of_source_point" ;
float Sources_Temp(Sources) ;
Sources_Temp:units = "Celcius_degree" ;
Sources_Temp:long_name = "Temperature_of_source_point" ;
float Sources_Height(Sources) ;
Sources_Height:units = "Meter" ;
Sources_Height:long_name = "Height_of_source_point" ;
float Sources_Diameter(Sources) ;
Sources_Diameter:units = "Meter" ;
Sources_Diameter:long_name = "Diameter_of_source_point" ;
float Sources_Velocity(Sources) ;
Sources_Velocity:units = "Meter/s" ;
Sources_Velocity:long_name = "Velocity_of_source_point_emission" ;
float NO2(Time, type_day, Sources) ;
NO2:units = "molecule/cm2/s" ;
NO2:long_name = "NO2 Emission" ;

// global attributes:
:Title = "CHIMERE SUITE" ;
:Sub-title = "Hourly point emission" ;
:Chimere_type = "EMISSIONS" ;
:Generating_process = "Generated by distribemis" ;
:Conventions = "None" ;
:Domain = "CONT5" ;
:Emission_version = "2008b" ;
:history = "" ;
}

G.2  exdomout.nc

netcdf exdomout {
dimensions:
  Time = UNLIMITED ; // (13 currently)
  DateStrLen = 19 ;
  west_east = 67 ;
  south_north = 46 ;
  bottom_top = 32 ;
variables:
  char Times(Time, DateStrLen) ;
  float lon(south_north, west_east) ;
lon:units = "degrees_east";
lon:long_name = "Longitude";
float lat(south_north, west_east);
lat:units = "degrees_north";
lat:long_name = "Latitude";
float sshf(Time, south_north, west_east);
sshf:units = "W/m^2";
sshf:long_name = "Surface sensible heat flux";
float slhf(Time, south_north, west_east);
slhf:units = "W/m^2";
slhf:long_name = "Surface latent heat flux";
float usta(Time, south_north, west_east);
uesta:units = "m/s";
uesta:long_name = "Frictional velocity";
float tem2(Time, south_north, west_east);
tem2:units = "K";
tem2:long_name = "2m air temperature";
float soim(Time, south_north, west_east);
soim:units = "m^3/m^3";
soim:long_name = "Soil Moisture level 1";
float hght(Time, south_north, west_east);
hght:units = "m";
hght:long_name = "PBL height from MM5";
float rh2m(Time, south_north, west_east);
rh2m:units = "fraction";
rh2m:long_name = "Relative Humidity at 2m";
float lspc(Time, south_north, west_east);
lspc:units = "kg/m^2";
lspc:long_name = "Large scale precipitation";
float copc(Time, south_north, west_east);
copc:units = "kg/m^2";
copc:long_name = "convective precipitation";
float u10m(Time, south_north, west_east);
u10m:units = "m/s";
u10m:long_name = "10 m U wind";
float v10m(Time, south_north, west_east);
v10m:units = "m/s";
v10m:long_name = "10 m V wind";
float temp(Time, bottom_top, south_north, west_east);
temp:units = "K";
temp:long_name = "Temperature";
float cliq(Time, bottom_top, south_north, west_east);
cliq:units = "kg/kg";
cliq:long_name = "Cloud liquid water mixing ratio";
float rain(Time, bottom_top, south_north, west_east);
rain:units = "kg/kg";
rain:long_name = "Rain water mixing ratio";
float sphu(Time, bottom_top, south_north, west_east);
sphu:units = "kg/kg";
sphu:long_name = "Specific humidity";
float cice(Time, bottom_top, south_north, west_east);
cice:units = "kg/kg";
cice:long_name = "Ice mixing ratio";
float pres(Time, bottom_top, south_north, west_east);
pres:units = "Pa";
pres:long_name = "Pressure";
float alti(Time, bottom_top, south_north, west_east);
alti:units = "m";
alti:long_name = "Altitude of half-sigma level";
float winz(Time, bottom_top, south_north, west_east);
winz:units = "m/s";
```csharp
winz:long_name = "Zonal wind";
float winm(Time, bottom_top, south_north, west_east);
winm:units = "m/s";
winm:long_name = "Meridional wind";

// global attributes:
:Title = "CHIMERE SUITE";
:Sub-title = "Interpolated Meteo file";
:Generating_process = "Generated by prepexmm5";
:Conventions = "";
:Domain = "CONT3";
:history = "File exdomout.nc was generated on",
"Tue Nov 15 14:25:27 2005 by <user> on <host>",
"from input file EUR1/MMOUT_EUR1_20030730_20030803_S\n";
:mm5_nxx = 85;
:mm5_nxx_DOT = 86;
:mm5_nyy = 75;
:mm5_nyy_DOT = 76;
:mm5_nlev = 32;
}

G.3 meteo.nc

netcdf meteo.20090312_20090319_test {
dimensions:
Time = UNLIMITED ; // (193 currently)
DateStrLen = 19;
west_east = 79;
south_north = 47;
bottom_top = 8;
variables:
float lon(south_north, west_east);
lon:units = "degrees_east";
lon:long_name = "Longitude";
float lat(south_north, west_east);
lat:units = "degrees_north";
lat:long_name = "Latitude";
char Times(Time, DateStrLen);
float hght(Time, south_north, west_east);
hght:units = "m";
hght:long_name = "Boundary layer height";
float u10m(Time, south_north, west_east);
u10m:units = "m/s";
u10m:long_name = "10m zonal wind speed";
float v10m(Time, south_north, west_east);
v10m:units = "m/s";
v10m:long_name = "10m meridional wind speed";
float w10m(Time, south_north, west_east);
w10m:units = "m/s";
w10m:long_name = "10m vertical wind speed";
float usta(Time, south_north, west_east);
uesta:units = "m/s";
uesta:long_name = "Friction velocity u*";
float wsta(Time, south_north, west_east);
wsta:units = "m/s";
wsta:long_name = "Convection velocity w*";
float tem2(Time, south_north, west_east);
tem2:units = "K";
tem2:long_name = "2m temperature";
float soim(Time, south_north, west_east);
```
soim:units = "m^3/m^3" ;
soim:long_name = "Soil moisture" ;
float sreh(Time, south_north, west_east) ;
sreh:units = "%" ;
sreh:long_name = "Surface relative humidity" ;
float psfc(Time, south_north, west_east) ;
psfc:units = "Pa" ;
psfc:long_name = "Surface pressure" ;
float sshf(Time, south_north, west_east) ;
sshf:units = "W/m2" ;
sshf:long_name = "Surface sensible heat flux" ;
float slhf(Time, south_north, west_east) ;
slhf:units = "W/m2" ;
slhf:long_name = "Surface latent heat flux" ;
float copc(Time, south_north, west_east) ;
copc:units = "mm/h" ;
copc:long_name = "Convective precipitation" ;
float lspc(Time, south_north, west_east) ;
lspc:units = "kg/m^2/h" ;
lspc:long_name = "Large scale precipitation" ;
float topc(Time, south_north, west_east) ;
topc:units = "kg/m^2/h" ;
topc:long_name = "Precipitation" ;
float aerr(Time, south_north, west_east) ;
aerr:units = "s/m" ;
aerr:long_name = "Aerodynamic resistance" ;
float atte(Time, south_north, west_east) ;
atte:units = "[0-1]" ;
atte:long_name = "Radiation attenuation factor" ;
float swrd(Time, south_north, west_east) ;
swrd:units = "W/m2" ;
swrd:long_name = "Shortwave radiation" ;
float winz(Time, bottom_top, south_north, west_east) ;
winz:units = "m/s" ;
winz:long_name = "Zonal wind" ;
float winm(Time, bottom_top, south_north, west_east) ;
winm:units = "m/s" ;
winm:long_name = "Meridional wind" ;
float winw(Time, bottom_top, south_north, west_east) ;
winw:units = "m/s" ;
winw:long_name = "Vertical wind" ;
float temp(Time, bottom_top, south_north, west_east) ;
temp:units = "K" ;
temp:long_name = "Temperature" ;
float sphu(Time, bottom_top, south_north, west_east) ;
sphu:units = "kg/kg" ;
sphu:long_name = "Specific humidity" ;
float airm(Time, bottom_top, south_north, west_east) ;
airm:units = "molecule/m**3" ;
airm:long_name = "Air density" ;
float hlay(Time, bottom_top, south_north, west_east) ;
hlay:units = "m" ;
hlay:long_name = "Layer top altitude" ;
float kzzz(Time, bottom_top, south_north, west_east) ;
kzzz:units = "m2/s2" ;
kzzz:long_name = "Kz diffusion coefficient" ;
float cliwc(Time, bottom_top, south_north, west_east) ;
cliwc:units = "kg/kg" ;
cliwc:long_name = "Liquid (+ice) water content" ;
float cliq(Time, bottom_top, south_north, west_east) ;
cliq:units = "kg/kg" ;
cliq:long_name = "Cloud liquid water mixing ratio";
float rain(Time, bottom_top, south_north, west_east);
rain:units = "kg/kg";
rain:long_name = "Rain water mixing ratio";
float pres(Time, bottom_top, south_north, west_east);
pres:units = "Pa";
pres:long_name = "Pressure";
float cice(Time, bottom_top, south_north, west_east);
cice:units = "kg/kg";
cice:long_name = "Ice liquid water mixing ratio";
float thlay(Time, bottom_top, south_north, west_east);
thlay:units = "m";
thlay:long_name = "Layer thickness";
float dpeu(Time, bottom_top, south_north, west_east);
dpeu:units = "kg/m²/s";
dpeu:long_name = "Entrainment in updraft";
float dpdu(Time, bottom_top, south_north, west_east);
dpdu:units = "kg/m²/s";
dpdu:long_name = "Detrainment in updraft";
float dped(Time, bottom_top, south_north, west_east);
dped:units = "kg/m²/s";
dped:long_name = "Entrainment in downdraft";
float dpdd(Time, bottom_top, south_north, west_east);
dpdd:units = "kg/m²/s";
dpdd:long_name = "Detrainment in downdraft";
float flxu(Time, bottom_top, south_north, west_east);
flxu:units = "kg/m²/s";
flxu:long_name = "updraft mass flux";
float flxd(Time, bottom_top, south_north, west_east);
flxd:units = "kg/m²/s";
flxd:long_name = "downdraft mass flux";

// global attributes:
:Title = "CHIMERE SUITE";
:Sub-title = "Hourly output meteo file";
:Chimere_type = "Chimere Meteo";
:Generating_process = "Generated by chimere";
:Conventions = "None";
:Domain = "CONT5";
:Chimere_version = "chimere2014b";
:history = "unknown";
}

G.4 AEMISSIONS.nc

netcdf AEMISSIONS {
dimensions:
Time = UNLIMITED ; // (24 currently)
west_east = 79 ;
south_north = 47 ;
bottom_top = 8 ;
SpStrLen = 23 ;
DateStrLen = 19 ;
Species = 24 ;

variables:
char Times(Time, DateStrLen) ;
char species(Species, SpStrLen) ;
float lon(south_north, west_east) ;
lon:units = "degrees_east" ;
lon:long_name = "Longitude";
float lat(south_north, west_east);
lat:units = "degrees_north";
lat:long_name = "Latitude";
float APIEN(Time, bottom_top, south_north, west_east);
APIEN:units = "molecule/cm2/s";
APIEN:long_name = "APIEN Emission";
float C2H4(Time, bottom_top, south_north, west_east);
C2H4:units = "molecule/cm2/s";
C2H4:long_name = "C2H4 Emission";
float C2H6(Time, bottom_top, south_north, west_east);
C2H6:units = "molecule/cm2/s";
C2H6:long_name = "C2H6 Emission";
float C3H6(Time, bottom_top, south_north, west_east);
C3H6:units = "molecule/cm2/s";
C3H6:long_name = "C3H6 Emission";
float C5H8(Time, bottom_top, south_north, west_east);
C5H8:units = "molecule/cm2/s";
C5H8:long_name = "C5H8 Emission";
float CH3CHO(Time, bottom_top, south_north, west_east);
CH3CHO:units = "molecule/cm2/s";
CH3CHO:long_name = "CH3CHO Emission";
float CH3COE(Time, bottom_top, south_north, west_east);
CH3COE:units = "molecule/cm2/s";
CH3COE:long_name = "CH3COE Emission";
float CH4(Time, bottom_top, south_north, west_east);
CH4:units = "molecule/cm2/s";
CH4:long_name = "CH4 Emission";
float CO(Time, bottom_top, south_north, west_east);
CO:units = "molecule/cm2/s";
CO:long_name = "CO Emission";
float HCHO(Time, bottom_top, south_north, west_east);
HCHO:units = "molecule/cm2/s";
HCHO:long_name = "HCHO Emission";
float HONO(Time, bottom_top, south_north, west_east);
HONO:units = "molecule/cm2/s";
HONO:long_name = "HONO Emission";
float NC4H10(Time, bottom_top, south_north, west_east);
NC4H10:units = "molecule/cm2/s";
NC4H10:long_name = "NC4H10 Emission";
float NH3(Time, bottom_top, south_north, west_east);
NH3:units = "molecule/cm2/s";
NH3:long_name = "NH3 Emission";
float NO(Time, bottom_top, south_north, west_east);
NO:units = "molecule/cm2/s";
NO:long_name = "NO Emission";
float NO2(Time, bottom_top, south_north, west_east);
NO2:units = "molecule/cm2/s";
NO2:long_name = "NO2 Emission";
float OXYL(Time, bottom_top, south_north, west_east);
OXYL:units = "molecule/cm2/s";
OXYL:long_name = "OXYL Emission";
float SO2(Time, bottom_top, south_north, west_east);
SO2:units = "molecule/cm2/s";
SO2:long_name = "SO2 Emission";
float H2SO4_fin(Time, bottom_top, south_north, west_east);
H2SO4_fin:units = "molecule/cm2/s";
H2SO4_fin:long_name = "H2SO4_fin Emission";
float PPM_big(Time, bottom_top, south_north, west_east);
PPM_big:units = "molecule/cm2/s";
PPM_big:long_name = "PPM_big Emission";
float PPM_coa(Time, bottom_top, south_north, west_east) ;
PPM_coa:units = "molecule/cm2/s" ;
PPM_coa:long_name = "PPM_coa Emission" ;
float OCAR_fin(Time, bottom_top, south_north, west_east) ;
OCAR_fin:units = "molecule/cm2/s" ;
OCAR_fin:long_name = "OCAR_fin Emission" ;
float BCAR_fin(Time, bottom_top, south_north, west_east) ;
BCAR_fin:units = "molecule/cm2/s" ;
BCAR_fin:long_name = "BCAR_fin Emission" ;
float TOL(Time, bottom_top, south_north, west_east) ;
TOL:units = "molecule/cm2/s" ;
TOL:long_name = "TOL Emission" ;
float TMB(Time, bottom_top, south_north, west_east) ;
TMB:units = "molecule/cm2/s" ;
TMB:long_name = "TMB Emission" ;

// global attributes:
>Title = "CHIMERE SUITE" ;
:Sub-title = "Emissions file - Surfacic + Point sources + Fires" ;
:Generating_process = "Generated by prepemis" ;
:Conventions = "" ;
:Domain = "CONT5" ;
:history = "" ;

G.5 BEMISSIONS.nc

netcdf BEMISSIONS {

dimensions:
Time = UNLIMITED ; // (13 currently)
DateStrLen = 19 ;
west_east = 67 ;
south_north = 46 ;
biospecies = 13 ;

variables:
    char Times(Time, DateStrLen) ;
    float lon(south_north, west_east) ;
    float lat(south_north, west_east) ;
    float C5H8(Time, south_north, west_east) ;
    float APINEN(Time, south_north, west_east) ;
    float BPINEN(Time, south_north, west_east) ;
    float LIMONE(Time, south_north, west_east) ;
    float TERPEN(Time, south_north, west_east) ;
    float OCIMEN(Time, south_north, west_east) ;
    float HUMULE(Time, south_north, west_east) ;
    float NO(Time, south_north, west_east) ;
    float SALT_coa(Time, south_north, west_east) ;
    float NA_coa(Time, south_north, west_east) ;
    float HCL_coa(Time, south_north, west_east) ;
    float H2SO4_coa(Time, south_north, west_east) ;
    float WATER_coa(Time, south_north, west_east) ;

// global attributes:
>Title = "CHIMERE SUITE" ;
:Sub-title = "Bioemissions file" ;
:Generating_process = "Generated by calbio" ;
:Conventions = "" ;
:Domain = "CONT3" ;
:history = "File BEMISSIONS.nc",
            "was generated on Tue Nov 15 14:25:40 2005 ",}
G.6 BOUN_CONCS.nc

```plaintext
netcdf BOUN_CONCS {

dimensions:
   Time = UNLIMITED ; // (121 currently)
   DateStrLen = 19 ;
   SpStrLen = 23 ;
   west_east = 101 ;
   south_north = 111 ;
   bottom_top = 20 ;
   h_boundary = 424 ;
   Species = 169 ;

variables:
   char Times(Time, DateStrLen) ;
   char species(Species, SpStrLen) ;
   float lon(south_north, west_east) ;
   float lat(south_north, west_east) ;
   float top_conc(Time, south_north, west_east, Species) ;
   float lat_conc(Time, bottom_top, h_boundary, Species) ;

// global attributes:
 :Title = "CHIMERE SUITE" ;
 :Sub-title = "Fine boundary concentrations file" ;
 :Generating_process = "Generated by prep_CHIMERE" ;
}
```

G.7 end.nc

```plaintext
netcdf end.20030730_20030803_heat-wave {

dimensions:
   Time = UNLIMITED ; // (1 currently)
   DateStrLen = 19 ;
   SpecStrLen = 16 ;
   Species = 119 ;
   west_east = 67 ;
   south_north = 46 ;
   bottom_top = 8 ;

variables:
   float lon(south_north, west_east) ;
   lon:units = "degrees_east" ;
   lon:long_name = "Longitude" ;
   float lat(south_north, west_east) ;
   lat:units = "degrees_north" ;
   lat:long_name = "Latitude" ;
   char species_name(Species, SpecStrLen) ;
   char Times(Time, DateStrLen) ;
   float APINEN(Time, bottom_top, south_north, west_east) ;
   APINEN:units = "molecules/cm3" ;
   float C2H4(Time, bottom_top, south_north, west_east) ;
   C2H4:units = "molecules/cm3" ;
   float C2H6(Time, bottom_top, south_north, west_east) ;
   C2H6:units = "molecules/cm3" ;
```
float C3H6(Time, bottom_top, south_north, west_east);
C3H6:units = "molecules/cm^3";
float C5H8(Time, bottom_top, south_north, west_east);
C5H8:units = "molecules/cm^3";
float C3HCHO(Time, bottom_top, south_north, west_east);
C3HCHO:units = "molecules/cm^3";
float C3HCOE(Time, bottom_top, south_north, west_east);
C3HCOE:units = "molecules/cm^3";
float C3HCOO(Time, bottom_top, south_north, west_east);
C3HCOO:units = "molecules/cm^3";
float C3HCOY(Time, bottom_top, south_north, west_east);
C3HCOY:units = "molecules/cm^3";
float C3H2O2(Time, bottom_top, south_north, west_east);
C3H2O2:units = "molecules/cm^3";
float C3H2O2H(Time, bottom_top, south_north, west_east);
C3H2O2H:units = "molecules/cm^3";
float C4H(Time, bottom_top, south_north, west_east);
C4H:units = "molecules/cm^3";
float CO(Time, bottom_top, south_north, west_east);
CO:units = "molecules/cm^3";
float DUSTAQ(Time, bottom_top, south_north, west_east);
DUSTAQ:units = "molecules/cm^3";
float GLYOX(Time, bottom_top, south_north, west_east);
GLYOX:units = "molecules/cm^3";
float H2O2(Time, bottom_top, south_north, west_east);
H2O2:units = "molecules/cm^3";
float H2SO4(Time, bottom_top, south_north, west_east);
H2SO4:units = "molecules/cm^3";
float H2SO4AQ(Time, bottom_top, south_north, west_east);
H2SO4AQ:units = "molecules/cm^3";
float HCHO(Time, bottom_top, south_north, west_east);
HCHO:units = "molecules/cm^3";
float HNO3(Time, bottom_top, south_north, west_east);
HNO3:units = "molecules/cm^3";
float HNO3AQ(Time, bottom_top, south_north, west_east);
HNO3AQ:units = "molecules/cm^3";
float HO2(Time, bottom_top, south_north, west_east);
HO2:units = "molecules/cm^3";
float HONO(Time, bottom_top, south_north, west_east);
HONO:units = "molecules/cm^3";
float ISNI(Time, bottom_top, south_north, west_east);
ISNI:units = "molecules/cm^3";
float MAC(Time, bottom_top, south_north, west_east);
MAC:units = "molecules/cm^3";
float MEMALD(Time, bottom_top, south_north, west_east);
MEMALD:units = "molecules/cm^3";
float MGLYOX(Time, bottom_top, south_north, west_east);
MGLYOX:units = "molecules/cm^3";
float MVK(Time, bottom_top, south_north, west_east);
MVK:units = "molecules/cm^3";
float N2O5(Time, bottom_top, south_north, west_east);
N2O5:units = "molecules/cm^3";
float NC4H10(Time, bottom_top, south_north, west_east);
NC4H10:units = "molecules/cm^3";
float NH3(Time, bottom_top, south_north, west_east);
NH3:units = "molecules/cm^3";
float NH3AQ(Time, bottom_top, south_north, west_east);
NH3AQ:units = "molecules/cm^3";
float NO(Time, bottom_top, south_north, west_east);
NO:units = "molecules/cm3" ;
float NO2(Time, bottom_top, south_north, west_east) ;
NO2:units = "molecules/cm3" ;
float NO3(Time, bottom_top, south_north, west_east) ;
NO3:units = "molecules/cm3" ;
float O3(Time, bottom_top, south_north, west_east) ;
O3:units = "molecules/cm3" ;
float obio(Time, bottom_top, south_north, west_east) ;
obio:units = "molecules/cm3" ;
float obioH(Time, bottom_top, south_north, west_east) ;
obioH:units = "molecules/cm3" ;
float OH(Time, bottom_top, south_north, west_east) ;
OH:units = "molecules/cm3" ;
float oPAN(Time, bottom_top, south_north, west_east) ;
oPAN:units = "molecules/cm3" ;
float oRN1(Time, bottom_top, south_north, west_east) ;
oRN1:units = "molecules/cm3" ;
float oRO2(Time, bottom_top, south_north, west_east) ;
oRO2:units = "molecules/cm3" ;
float oROOH(Time, bottom_top, south_north, west_east) ;
oROOH:units = "molecules/cm3" ;
float OXYL(Time, bottom_top, south_north, west_east) ;
OXYL:units = "molecules/cm3" ;
float PAN(Time, bottom_top, south_north, west_east) ;
PAN:units = "molecules/cm3" ;
float PANH(Time, bottom_top, south_north, west_east) ;
PANH:units = "molecules/cm3" ;
float PPA(Time, bottom_top, south_north, west_east) ;
PPA:units = "molecules/cm3" ;
float PPMAQ(Time, bottom_top, south_north, west_east) ;
PPMAQ:units = "molecules/cm3" ;
float SO2(Time, bottom_top, south_north, west_east) ;
SO2:units = "molecules/cm3" ;
float SOA(Time, bottom_top, south_north, west_east) ;
SOA:units = "molecules/cm3" ;
float SOAAQ(Time, bottom_top, south_north, west_east) ;
SOAAQ:units = "molecules/cm3" ;
float toPAN(Time, bottom_top, south_north, west_east) ;
toPAN:units = "molecules/cm3" ;
float p1PPM(Time, bottom_top, south_north, west_east) ;
p1PPM:units = "molecules/cm3" ;
float p1DUST(Time, bottom_top, south_north, west_east) ;
p1DUST:units = "molecules/cm3" ;
float p1SOA(Time, bottom_top, south_north, west_east) ;
p1SOA:units = "molecules/cm3" ;
float p1H2SO4(Time, bottom_top, south_north, west_east) ;
p1H2SO4:units = "molecules/cm3" ;
float p1HNO3(Time, bottom_top, south_north, west_east) ;
p1HNO3:units = "molecules/cm3" ;
float p1NH3(Time, bottom_top, south_north, west_east) ;
p1NH3:units = "molecules/cm3" ;
float p1WATER(Time, bottom_top, south_north, west_east) ;
p1WATER:units = "molecules/cm3" ;
float p2PPM(Time, bottom_top, south_north, west_east) ;
p2PPM:units = "molecules/cm3" ;
float p2DUST(Time, bottom_top, south_north, west_east) ;
p2DUST:units = "molecules/cm3" ;
float p2SOA(Time, bottom_top, south_north, west_east) ;
p2SOA:units = "molecules/cm3" ;
float p2H2SO4(Time, bottom_top, south_north, west_east) ;
p2H2SO4:units = "molecules/cm3" ;

float p2HNO3(Time, bottom_top, south_north, west_east);
p2HNO3:units = "molecules/cm3";
float p2NH3(Time, bottom_top, south_north, west_east);
p2NH3:units = "molecules/cm3";
float p2WATER(Time, bottom_top, south_north, west_east);
p2WATER:units = "molecules/cm3";
float p3PPM(Time, bottom_top, south_north, west_east);
p3PPM:units = "molecules/cm3";
float p3DUST(Time, bottom_top, south_north, west_east);
p3DUST:units = "molecules/cm3";
float p3SOA(Time, bottom_top, south_north, west_east);
p3SOA:units = "molecules/cm3";
float p3H2SO4(Time, bottom_top, south_north, west_east);
p3H2SO4:units = "molecules/cm3";
float p3HNO3(Time, bottom_top, south_north, west_east);
p3HNO3:units = "molecules/cm3";
float p3NH3(Time, bottom_top, south_north, west_east);
p3NH3:units = "molecules/cm3";
float p3WATER(Time, bottom_top, south_north, west_east);
p3WATER:units = "molecules/cm3";
float p4PPM(Time, bottom_top, south_north, west_east);
p4PPM:units = "molecules/cm3";
float p4DUST(Time, bottom_top, south_north, west_east);
p4DUST:units = "molecules/cm3";
float p4SOA(Time, bottom_top, south_north, west_east);
p4SOA:units = "molecules/cm3";
float p4H2SO4(Time, bottom_top, south_north, west_east);
p4H2SO4:units = "molecules/cm3";
float p4HNO3(Time, bottom_top, south_north, west_east);
p4HNO3:units = "molecules/cm3";
float p4NH3(Time, bottom_top, south_north, west_east);
p4NH3:units = "molecules/cm3";
float p4WATER(Time, bottom_top, south_north, west_east);
p4WATER:units = "molecules/cm3";
float p5PPM(Time, bottom_top, south_north, west_east);
p5PPM:units = "molecules/cm3";
float p5DUST(Time, bottom_top, south_north, west_east);
p5DUST:units = "molecules/cm3";
float p5SOA(Time, bottom_top, south_north, west_east);
p5SOA:units = "molecules/cm3";
float p5H2SO4(Time, bottom_top, south_north, west_east);
p5H2SO4:units = "molecules/cm3";
float p5HNO3(Time, bottom_top, south_north, west_east);
p5HNO3:units = "molecules/cm3";
float p5NH3(Time, bottom_top, south_north, west_east);
p5NH3:units = "molecules/cm3";
float p5WATER(Time, bottom_top, south_north, west_east);
p5WATER:units = "molecules/cm3";
float p6PPM(Time, bottom_top, south_north, west_east);
p6PPM:units = "molecules/cm3";
float p6DUST(Time, bottom_top, south_north, west_east);
p6DUST:units = "molecules/cm3";
float p6SOA(Time, bottom_top, south_north, west_east);
p6SOA:units = "molecules/cm3";
float p6H2SO4(Time, bottom_top, south_north, west_east);
p6H2SO4:units = "molecules/cm3";
float p6HNO3(Time, bottom_top, south_north, west_east);
p6HNO3:units = "molecules/cm3";
float p6NH3(Time, bottom_top, south_north, west_east);
p6NH3:units = "molecules/cm3";
float p6WATER(Time, bottom_top, south_north, west_east);
units = "molecules/cm3";
float M(Time, bottom_top, south_north, west_east);
M:units = "molecules/cm3";
float O2(Time, bottom_top, south_north, west_east);
O2:units = "molecules/cm3";
float N2(Time, bottom_top, south_north, west_east);
N2:units = "molecules/cm3";
float H2O(Time, bottom_top, south_north, west_east);
H2O:units = "molecules/cm3";
float TOTPAN(Time, bottom_top, south_north, west_east);
TOTPAN:units = "molecules/cm3";
float NOX(Time, bottom_top, south_north, west_east);
NOX:units = "molecules/cm3";
float OX(Time, bottom_top, south_north, west_east);
OX:units = "molecules/cm3";
float NOY(Time, bottom_top, south_north, west_east);
NOY:units = "molecules/cm3";
float ROCO2H(Time, bottom_top, south_north, west_east);
ROOH:units = "molecules/cm3";
float HCNM(Time, bottom_top, south_north, west_east);
HCNM:units = "molecules/cm3";
float PM10(Time, bottom_top, south_north, west_east);
PM10:units = "molecules/cm3";
float PM25(Time, bottom_top, south_north, west_east);
PM25:units = "molecules/cm3";
float PM10_anth(Time, bottom_top, south_north, west_east);
PM10_anth:units = "molecules/cm3";
float PM25_anth(Time, bottom_top, south_north, west_east);
PM25_anth:units = "molecules/cm3";
float PPM10_anth(Time, bottom_top, south_north, west_east);
PPM10_anth:units = "molecules/cm3";
float PPM25_anth(Time, bottom_top, south_north, west_east);
PPM25_anth:units = "molecules/cm3";
float pPPM(Time, bottom_top, south_north, west_east);
pPPM:units = "molecules/cm3";
float pDUST(Time, bottom_top, south_north, west_east);
pDUST:units = "molecules/cm3";
float pSOA(Time, bottom_top, south_north, west_east);
pSOA:units = "molecules/cm3";
float pH2SO4(Time, bottom_top, south_north, west_east);
pH2SO4:units = "molecules/cm3";
float pHNO3(Time, bottom_top, south_north, west_east);
pHNO3:units = "molecules/cm3";
float pNH3(Time, bottom_top, south_north, west_east);
pNH3:units = "molecules/cm3";
float pWATER(Time, bottom_top, south_north, west_east);
pWATER:units = "molecules/cm3";

// global attributes:
>Title = "CHIMERE SUITE";
:Sub-title = "Final concentrations file";
:Chimere_type = "end";
:Generating_process = "Generated by chimere";
:Conventions = "None";
:Domain = "CONT3";
:history = "File end.20030730_20030803_heat-wave.nc",
"was generated on Tue Nov 8 12:27:58 2005",
"by <user> on <host>\n";
G.8 Fire emissions EMIS.[domain].[MM].[SPEC].f.nc

netcdf EMIS.MEDa.06.CO.f {
  dimensions:
    west_east = 119 ;
    south_north = 84 ;
    days = 30 ;
    hours = 24 ;
    sources = 315 ;
  variables:
    float lon(south_north, west_east) ;
      lon:units = "degrees_east" ;
      lon:long_name = "Longitude" ;
    float lat(south_north, west_east) ;
      lat:units = "degrees_north" ;
      lat:long_name = "Latitude" ;
    float ilatsources(sources) ;
      ilatsources:units = "index" ;
      ilatsources:long_name = "Latitude_of_sources" ;
    float ilonsources(sources) ;
      ilonsources:units = "index" ;
      ilonsources:long_name = "Longitude_of_sources" ;
    float CO(hours, days, sources) ;
      CO:units = "molecule/cm2/s" ;
      CO:long_name = "CO Emission" ;
}