

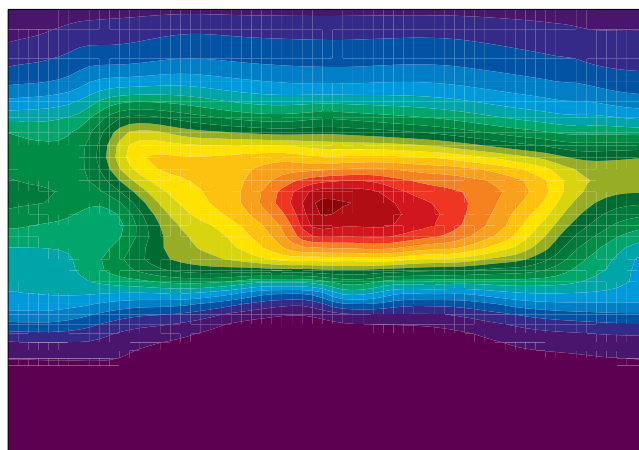
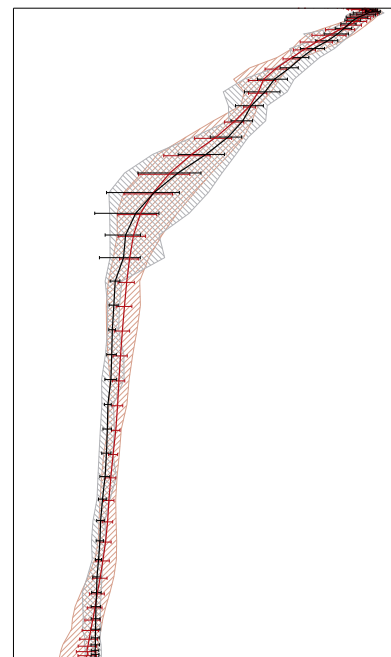
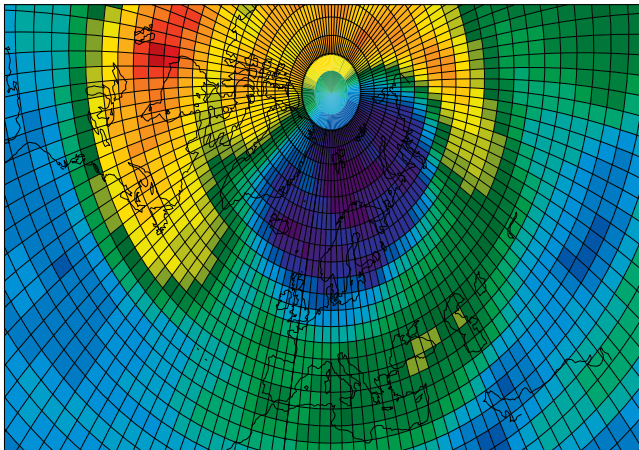
Oslo CTM3

v1.0

User manual

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Abstract

This manual contains a description of the Oslo CTM3 and how to set up simulations. Information about emissions, which type of simulation you want do, with which components etc. are described, but most of all, this manual attempts to document the different processes and the source code of the Oslo CTM3.

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1 Oslo CTM3 manual

The Oslo CTM3 is a three dimensional global chemical transport model (CTM), and this manual explains how to use it. This manual also describes the model, and is meant as a thorough description of the model.

Generally, the use of the model is described in Section 2–5, while the rest is describing the different processes and the model code.

The Oslo CTM3 is available through a repository, as will be explained in the coming sections.

First, some starting info about the Oslo CTM3.

1.1 Historical background

Oslo CTM3 is developed at the Department of Geosciences at the University of Oslo (UiO), and later at the CICERO Center for International Climate Research. It is described by Søvde et al. (2012) and is an updated version of the Oslo CTM2, which was based on a CTM from University of California, Irvine (UCI), developed by Michael Prather & Xin Zhu (January 1996, p-code 1.0/96), and where the chemical modules developed at the UiO were included.

In roughly a decade the two models diverged substantially; the Oslo CTM2 grew with additional chemistry/aerosol packages, while the UCI group developed and improved the efficiency of the transport. In order to save CPU hour requirements, the UCI group (Prather *et al.*) updated their CTM to improve the structure, parallelisation and transport in 2007. Due to the large CPU requirements for the Oslo CTM2, it was decided to implement the new UCI structure in the Oslo model, earning the name Oslo CTM3.

By the end of 2007, the Oslo CTM2 was very messy, so the update of the core structure also initiated a clean-up of the Oslo CTM2 code.

1.2 Version numbering

The Oslo CTM3 documented by Søvde et al. (2012) is to be considered version v0.1, while the current version is v1.0. Version numbering is not directly related to repository revision numbers, however, in the Oslo CTM3 repository, the version documented by Søvde et al. (2012) was r143.

There are numerous small changes from version v0.1 to v1.0, e.g. that the aerosol packages have undergone some revisions, and the scavenging tables have been modified.

1.3 Oslo CTM3 vs the UCI CTM

During the first five years of Oslo CTM3 development, the basic idea of the Oslo CTM3 was to keep the UCI model core untouched, only adding modules we want and thereby staying away from interfering too much with the core.

However, in 2015, the UCI CTM had already diverged some bit from the starting point of Oslo CTM3, being partly rewritten to use modules instead of common blocks. So I decided to rewrite the Oslo CTM3 into fortran90. This was done for all files except the transport routines, which are the basis for the transport model. Keeping those intact may be wise in case of future UCI updates. However, all the common blocks are now gone.

The model driver (pmain) is kept clean and short; the Oslo CTM2 philosophy that all goes into pmain is left for good!

So far the Oslo CTM3 changes have been large enough so it is not possible to use the UCI chemistry just by operating a switc. The original UCI code files are available through the UCI group, and will not be available in

CTM3. I do, however, have their older codes if update history is needed.

1.4 Limitations to Oslo CTM3

Oslo CTM3 is a good tool to study the atmospheric processes. However, care should be taken when comparing model results with observations. Even a high resolution in the Oslo CTM3 is actually fairly coarse, so a perfect fit with observations, especially close to the Earth surface, should not be expected.

The Oslo CTM3 is primarily set up to study current meteorology, so when using it in pre-industrial conditions you have to make assumptions.

2 Get started

The Oslo CTM3 is currently available through a SVN repository (see Section 2.1), and to get access to the model you have to have a user account at the Department of Geosciences or at CICERO, and you have to be member of the unix group **gf-ozone**. This will change eventually.

I have planned to eventually make the Oslo CTM3 open source, but that is yet for the future.

When you are well into the model, you may need some utilities or programs (for generating e.g. input files). Such CTM-files may not be part of the SVN, and may otherwise be located at `/div/amoc/d4-4/oslo-ctm/archive_ctm/`.

Part of the SVN, though, are some tools for post processing. More of this later.

In this Section you will find a short description of how to download the model from the SVN repository, a short model overview and how to get it running.

2.1 How to get the model – SVN

The Oslo CTM3 is available through the UiO central sub-version system (SVN). To access the code you have to be member of the group **gf-ozone**.

SVN is a version control system, and if you are unfamiliar with it, the SVN book offers a fairly good introduction to it: <http://svnbook.red-bean.com/>.

To use SVN you need to have SVN installed/loaded. Contact your IT services if you need help on this.

Important SVN commands are **checkout**, **add**, **delete**, **commit**, **status**, **diff**, **resolve** (for versions prior to 1.5 it is called **resolved**).

You will find more about SVN in the SVN book, and a short summary in Appendix B. The repository structure is described in Section B.1, where you will also see that there also are some plotting utilities and other tools available.

Fetching the code

The code is located in a repository, and you get it by typing (in shell scripts, `'\'` allows you to write a command on several lines; you should skip character that and write everything on one line):

```
svn checkout \
  svn+ssh://svn.uio.no/svnroot/osloctm3/ctm3f90 \
  <name of dir to put the code>
```

After doing this, you have a copy of the code in the directory you specified. In the `.svn` directory the original revision files are also available, but you will not use those directly; `.svn` is for SVN to use.

If you don't specify the name of directory where the code will be copied to, it will get the repository name, i.e. `ctm3f90`.

Update an existing code

If one of the experienced users tell you to update your code, just go to your directory and execute the command:

```
svn update
```

Note that if you have modified a file that needs update, you may experience a conflict, i.e. SVN does not understand how to merge the changes. If you are unfamiliar with this, ask the experienced users.

2.2 User manual

The Oslo CTM3 user manual (this document) is available as a pdf file (*manual_osloctm3.pdf*) in the model directory. The L^AT_EX source code is located in a separate repository.

2.3 Source code directory

When you have downloaded the source code, you find that it contains several files and some directories. The transport source codes, i.e. the UCI heritage of the model, are located at the top level of the directory. Most of the files have the extension `.f90`, except for a few of the transport subroutines which have extension `.f`.

All the specific Oslo chemistry/physics files are put in the directory `OSLO`. You can find more about the directory structure in Appendix B.1, and in Appendix A you can find more information on the files.

2.4 Model grid

As already noted, the Oslo CTM3 is a global model. It is divided into grid boxes to cover the atmosphere and hence has a certain resolution. When you specify a resolution, there are three numbers to keep in mind, at least for ECMWF meteorology data. The truncation number is given by 'T' (e.g. T159), indicating the spectral resolution of the native model (e.g. ECMWF IFS). The vertical resolution is given by 'L' (L60). A forecast model can

have both gridded data and spectral data, in different resolutions, so to define the gridded data there is the 'N' number (N80). At ECMWF the T and N numbers are closely connected. See Appendix H for more.

In the Oslo CTM3 the spatial resolution is controlled by the following parameters:

- **IPAR**: Number of grid boxes in the zonal (east-west) direction. **IPARW** is the zonal resolution of the meteorological input data and differs from **IPAR** if you run with “degraded” horizontal resolution (see Section 2.4.1 for more on degradation of resolution).
- **JPAR**: Number of grid boxes in the meridional (north-south) direction. **JPARW** is the meridional resolution of the meteorological input data and differs from **JPAR** if you run with degraded horizontal resolution (see Section 2.4.1 for more on degradation of resolution).
- **LPAR**: Number of grid boxes in the vertical. If you collapse layers, the vertical resolution of the meteorological input data is **LPARW** (see Section 2.4.1 for more on collapsing layers).

There are several variables describing the grid. The horizontal grid is set up at model start, with grid center longitudes defined in:

- **XGRD (IPAR)**: Radians.
- **XDGRD (IPAR)**: Degrees.

And grid center latitudes:

- **YGRD (JPAR)**: Radians.
- **YDGRD (JPAR)**: Degrees.

The grid edges are defined similarly by:

- **XEDG (IPAR+1)**: Eastern edge longitude of grid box (radians).
- **XDEDG (IPAR+1)**: Eastern edge longitude of grid box (degrees).
- **YEDG (JPAR+1)**: Southern edge latitude of grid box (radians).
- **YDEDG (JPAR+1)**: Southern edge latitude of grid box (degrees).

The vertical grid, however, is not fixed throughout a model run. It depends on the meteorological input data, more specifically the pressure. For a model layer L , the pressure at the grid box bottom is given by

$$p_b(L) = \eta_a(L) + \eta_b(L) p_s \quad (1)$$

where p_s is surface pressure in hPa and η_a (**ETAA (LPAR+1)**, units of hPa) and η_b (**ETAB (LPAR+1)**, unitless) are hybrid sigma coordinates. If you collapse layers, the original sigma coordinates are given by **ETAAW (LPARW+1)** and **ETABW (LPARW+1)**.

The grid box center pressure of a level L is halfway between the edges of the box:

$$p_c(L) = \frac{1}{2} [\eta_a(L) + \eta_a(L+1) + (\eta_b(L) + \eta_b(L+1)) * p_s] \quad (2)$$

The height of grid box bottoms are given by the array **ZOFLE (LPAR+1, IPAR, JPAR)**. Surface values of this variable act as topography, and are calculated from a 2D annual mean surface pressure field p_m :

$$Z_s = 16000 \log_{10} \left(\frac{1013.25 \text{ hPa}}{p_m} \right) \quad (3)$$

The height levels above the surface (i.e. for the vertical range **2:LPAR+1** of **ZOFLE**) are calculated from the thickness of each layer, based on temperature (T), specific humidity (q) and pressure at grid box edges (p_b).

$$\Delta Z(L) = -29.27 T(L) [1 - 0.6 q(L)] \cdot \log \left(\frac{p_b(L+1)}{p_b(L)} \right) \quad (4)$$

Although Z_s is the topography in meters, this quantity is mainly used for diagnostics. Physical processes generally use **ZOFLE** to find layer thickness, while it is the surface pressure that defines the topography. See Appendix C.2 for some more info.

2.4.1 Degraded resolution

The Oslo CTM3 can be run with lower resolution than the meteorological input data. It is possible to collapse as many layers as you like, however, *Makefile* allows for only one automatic set-up, collapsing layer 1–3 and 4–5 into two layers. See Section 2.7.1 for *Makefile* user settings. While this is standard treatment by the UCI group, the Oslo CTM3 has so far not been used in this fashion.

A newer feature to Oslo CTM3 is that the horizontal resolution may be degraded, combining e.g. 4 boxes into one. This means that the model can read e.g. $1.125^\circ \times 1.125^\circ$ meteorological data, and convert them to $2.25^\circ \times 2.25^\circ$ resolution, but still using the native resolution for calculating cloud properties. The *Makefile* settings are:

- **HWINDOW=HORIGINAL**: Use native resolution.
- **HWINDOW=HTWO**: Combine 2×2 native boxes.
- **HWINDOW=HFOUR**: Combine 4×4 native boxes.

Also described in Section 2.7.1.

2.5 Oslo CTM3 vs Oslo CTM2

Skip this part if you are not familiar with Oslo CTM2.

The structure of the model has changed substantially since Oslo CTM2. In the Oslo CTM2 all tracers were located in the tracer array **STT**, whereas in Oslo CTM3 only the transported tracers are in **STT**. Therefore also **MTC** is now only for the transported species. Other variables have also been changed to separate the transported and non-transported species. The non-transported species are stored in **XSTT**, and will be further explained in Section 3.

The parallel structure has changed, and most processes (chemistry, boundary layer mixing, emissions, etc.) are now integrated columnwise instead of through a latitude band. Horizontal transport, however, is calculated layer by layer (see Section 6). Section 3 describes the source code more closely.

Input files and diagnostics

The diagnostics have changed, as well as the names of the input files. The input files are described in Section 2.7, while diagnostics are described in Section 21.

C-code

The C-coding in the Oslo CTM2 has been removed, and

replaced with dummy calls and logical switches. This will be explained thoroughly in this manual.

Changes in chemistry

There are some changes in the tracer list since Oslo CTM2:

- Tracer number 2 (NOX), the sum of NOx components (NO, NO₂, NO₃, 2xN₂O₅+PAN) is only set in the tropospheric chemistry for stability. There is no need to transport NOX since all its components are transported.
- Tracer number 3 (NOZ), the sum of NO₃ and N₂O₅ is removed. It is now set in the tropospheric chemistry, as was done already in the stratospheric chemistry. NOZ is treated in chemistry to create stability, and does not need to be transported as long as NO₃ and N₂O₅ are transported.
- Tracer number 26 (CH2020H) was transported but not used. It is removed.
- Tracer number 45 (O3N0) is set inside the tropospheric chemistry from O₃ and NO, also for stability. It was not transported, not used in the stratosphere, and the diagnose was not useful, therefore it was removed.
- Tracer number 47 (DMS) is not in use in the tropospheric chemistry, and is removed. It is used in the sulphur scheme where it has a new number (which is 71).

NPAR

In contrast to the Oslo CTM2 the STT now *only handles the transported species*, given by NPAR. Non-transported species are treated as a separate array XSTT, of which there are NOTRPAR. See Section 3.1 for more on this.

Convective activity

The convectivity files used for lightning emission in Oslo CTM2 are not needed in the Oslo CTM3. This is because the lightning routine is now more consistent with the meteorological data, not using the Price et al. (1997) dataset.

In the Oslo CTM3 we calculate a somewhat similar convective activity at each time step and scale it against a climatological mean. This mean is specific for a certain meteorological dataset, and is sensitive for resolution. An important difference to the Oslo CTM2 is that the Oslo CTM2 divided the annual amount following the monthly totals of Price et al. (1997), whereas Oslo CTM3 more physically follows only the meteorological conditions. It could be noted that Murray et al. (2012) argue that Northern Hemisphere summer lightning produce more NOx than elsewhere and at other seasons, but this is not included in Oslo CTM3. See Section 8.8 for more on lightning emissions.

fast-JX

The Fast-J2 (Bian and Prather, 2002) applied in the Oslo CTM2 has been replaced by fast-JX in the Oslo CTM3. There are some differences in the photochemistry, e.g. slight differences in cross sections.

Source code documentation

In the process of cleaning up the Oslo code, also the source code comments have been revised and improved. See Section 5 for programming guidelines.

Variable names

There are several variable names that have been renamed

from Oslo CTM2 to Oslo CTM3. The new variable names are more self-explaining.

A good example of a changed variable name is the tropopause level, which is now called LMTROP, since it is the “LM of the troposphere”. In the old model its name was LMSTRT, which was somewhat misleading.

Another is the max number of component IDs, which has been changed from IREPMX to TRACER_ID_MAX.

The tracer mapping from chemical id to transport number has changed name from MTC to `trsp_idx`. Similarly, the mapping the other way is changed from IDMTX to `chem_idx`.

TMVV, the conversion factor from mass mixing ratio to volume mixing ratio, is called TMASSMIX2MOLMIX. There are also mappings the other way, namely TMOLMIX2MASSMIX.

Old variable names are not listed in the index list, so if you wonder where to find the old variable, ask the experienced users.

Other differences

In the Oslo CTM2 the whole tracer array (STT) was often converted from one unit to another unit, just to access a few tracers in the correct units. This is no longer possible, and should be avoided.

Other differences are noted when necessary in the other sections.

2.6 Variable names

Most of the model variable names referred to in this manual are listed in the index list at the end of the manual, under “variables”. If you cannot find the variable names there, they are probably not mentioned here, and you have to look in the model files. A good place to start is the global variables in the files called `cmn_*` (cmn for common files instead of common blocks).

If you look for a variable and do not find it in the indexed list, you may also do a text search in this document; the variable may not have been included in the index list.

2.7 Setting up the model

This section will explain the steps to get the model running, and will describe some important files.

You need to know the

- Makefile
- `pmain.f90`
- input file (*LxxCTM.inp*), which lists some important flags and input file names.
- tracer list (*tracer_list.d*)
- wet scavenging list (*scavenging_wet.dat*), which lists how to treat wet scavenging of tracers.
- dry scavenging list (*scavenging_dry.dat*), which lists how UCI treats dry deposition of tracers. NOT used for Oslo chemistry! Oslo chemistry uses the file *dry-dep.ctm*, located in the directory *Input_CTM3*.
- meteorological data

- other input data, e.g. how to treat CH₄ at the surface (and possibly how to initialize the tracer array STT).

2.7.1 Makefile

The first file you need to know, is the *Makefile*. In *Makefile* you can set user options, i.e. which modules or packages to apply, which resolution to use and some compiler options. Your choices are:

- **OPTS**: Optimize (0, A) or debug (D).
- **HNATIVE**: Horizontal resolution of meteorological data, e.g. T42, T159.
- **VNATIVE**: Vertical resolution of meteorological data, most likely L60, but old files exist in e.g. L40.
- **HWINDOW**: Model degradation of horizontal resolution. Setting it to **HORIGINAL**, the model uses native resolution, and with **HTWO** it combines 2x2 native grid boxes. A third option is **HFOUR**.
- **COLLAPSE**: Collapse layer 1-3 and 4-5 into two layers.
- **OSLOCHEM**: Turn on Oslo chemistry/physics. For Oslo CTM3 you would most likely never turn this off.
- **TROPICHEM**: Oslo tropospheric chemistry (Section 10).
- **STRATCHEM**: Oslo stratospheric chemistry (Section 11).
- **SULPHUR**: Sulphur chemistry and sulphate (Section 13).
- **BCOC**: Black and organic carbon package (Section 14).
- **NITRATE**: Nitrate package (Section 17).
- **SEASALT**: Sea salt package (Section 16).
- **DUST**: Mineral dust package (Section 15).
- **SOA**: Secondary organic aerosols package (Section 19).
- **E90**: Turn on to use e90 tracer for STE flux calculations (Section 21.1.4) and to produce the tropopause **LSTRATAIR_E90** (not yet used to distinguish tropospheric and stratospheric chemistry).
- **LINOZ**: Turn on to use Linoz O₃ for STE calculations. Oslo CTM3 has not yet been set up to use Linoz to replace stratospheric chemistry.
- **LIT**: Can be used for generating lightning factors. Explanation is given in *Makefile*.
- **EMISDEP_TREATMENT**: Defines whether to treat emissions and deposition as separate processes (**EMISDEP_TREATMENT :=U**) or as respectively production and loss in chemistry (**EMISDEP_TREATMENT :=0**).
- **FC**: Fortran compiler (**ifort**, **pgf90**, **openf90** ...) See Appendix E for more on the compiler options.

Makefile does *not* use a dependency generator, so if you add files to be compiled you have to add dependency rules at the end of *Makefile*. How to do this is described closer in Appendix C.4.

The *Makefile* tokens set up the compilation and is used for setting model parameters. The file *cmn_size.F90* is the only file (except the mineral dust code) containing C-style code, and thereby needs to be preprocessed by the Fortran compiler.

See Section 2.8 if you don't know how to compile.

If you want to run non-standard resolutions, you need to check that the *cmn_size.F90* has the necessary parameters.

See Appendix C.4 for more on *Makefile*.

2.7.2 Main program – pmain

The main program is located in *pmain.f90*. It is described in Section 4. You should know the structure of *pmain.f90*, and how it works. When you need to work on the tracer arrays, you should also know how the parallel regions work.

2.7.3 Input file – LxxCTM.inp

There is one input file for each resolution, and it is typically called *LxxCTM.inp*. The first part of the file is to set up the run, with information about the date, time steps, meteorological fields, and physical processes (boundary layer mixing, dry and wet deposition schemes).

The second part lists some input file names, e.g. the tracer list (*tracer_list.d*), while the third part covers information about the diagnostics (covered in Section 21).

The important parameters to set are

- **IYEAR**: Reference year.
- **NDAYI**: Day of year to begin CTM run.
- **NDAYE**: Day at end of CTM run (finishes at end of day **NDAYE-1**).
- **LCLDQMD**: Use mid-point of quadrature cloud cover independent cloud atmospheres (ICA) (for fast-JX, Section 12.2).
- **LCLDQMN**: Mean quadrature cloud cover ICAs (for fast-JX).
- **LCLDRANA**: Random selected from all cloud cover ICAs (for fast-JX; default treatment).
- **LCLDRANQ**: Random selected from 4 mean quadrature cloud cover ICAs (for fast-JX).
- **RANSEED**: The seed number to create random numbers. Ensures that the random cloud properties are the same in two runs).
- **NROPSM**: Number of operator split steps per meteorological time step. Default is 1 hour, i.e. **NROPSM=3**. Note that the meteorological steps per day (**NRMETD**) is hard coded into the model because it is necessary for e.g. the diagnostic tools.
- **NRCHEM**: Number of chemical sub steps per operator split step. Default is **NRCHEM=1**.
- **LJCCYC**: Flag for calculating J-values every internal chemical cycling step. See Section 12 for more.
- **LMTSOM**: Second order moment limiter. Should be 2 (monotonic), but can also be set to 1 () and 3 (min/max). Do **not** change this unless you know what you are doing.
- **CFLIM**: Global CFL limit for divergence, i.e. max allowed amount taken from a grid box in advection. This value should be set to 0.95, and you should not need to change it. With the Oslo CTM2 there were a few instances where certain meteorological data would cause the model to crash because 0.95 was too high, this behaviour has so far not been seen in Oslo CTM3.

Next, there is a section for meteorological data, specifying which type of data and where to read them:

- **metTYPE:** Possible types are `ECMWF_oIFS` for OpenIFS generated locally at CICERO/UIO, and `ECMWF_IFS` for the IFS data generated at ECMWF/UIO.
- **metCYCLE:** The cycle of the ECMWF IFS/OpenIFS model.
- **metREVN:** The revision number of the ECMWF IFS/OpenIFS model.
- **LLPYR:** Allow for leap year.
- **LFXMET:** Annually recycle met fields.
- **JMPOLAR:** Defines if polar grid box has same latitudinal size as other grid boxes (`JMPOLAR=0`) or half size (`JMPOLAR=1`). Should be 0 for ECMWF data.
- **GM0000:** I-coord of Greenwich Meridian. For ECMWF `GM0000=1.5`, meaning that Greenwich (0°E) is in the middle of grid box 1 (so that 1 is left edge and 2 is right edge). Other meteorological data may have different grids.

After this, the hybrid sigma coordinates are listed. Note that if you collapse layers (`COLLAPSE` in *Makefile*), the `LMMAP` must match this. So if you collapse layers 1–3, the `LMMAP` of the first 3 entries must be 1. Native level 4 will then have `LMMAP=2`. Traditionally, the Oslo CTM3 had always been run in native vertical resolution, while UCI-CTM is often run with collapsed layers near the surface.

Next:

- **PFZON:** Allows polar latitudes to combine grid boxes horizontally. However, this is not applied in Oslo CTM3. Entries should therefore be 1 (there are 25 entries).
- **NBLX:** Boundary layer scheme (Section 6.4). Default should be 5.
- **NDPX:** Dry deposition scheme (Section 7.2). Only simple UCI scheme is available, but it is modified/overwritten for the Oslo CTM3.
- **NSCX:** Scavenging scheme for large scale scavenging (Section 7.1.1). Should be set to 1.

Then input filenames for annual mean pressure and vegetation are listed, followed by more tracer specific parameters, e.g. how to start the model:

- **LCONT:** Start from restart file (T) or not (F).
- **START_AVG:** If `LCONT = F`, this index specifies how else to initialize the tracer field. `START_AVG=0`: `STT=0`, `START_AVG=1`: start from Oslo CTM3 average file.

In this tracer specific section, the filenames of the tracer list (Section 2.7.4), scavenging lists and emission list (Section 2.7.5) are given.

Note that the tracer list is read immediately after it is defined. This is to allow for checking against included tracers, e.g. by different diagnostics.

Lastly, there are several settings and flag calendars for diagnostics.

- **JDO_C:** When to save restart files.
- **JDO_T:** When to do tendencies.

With the tendency tracer flags you specify which tracers to diagnose. Note that these are transport numbers, not component IDs.

Then we have:

- **JDO_A:** When to do averages.
- **JDO_X:** When to do STE calculations.

And finally the UCI time series output. This is not the same as the Oslo CTM3 time series (Section 21.2.6), and is not used.

Future update

Using transport numbers to define output is problematic, because you need to keep track of the order of components. In the future this will be changed to component names.

2.7.4 Tracer list – *tracer_list.d*

The tracer list (*tracer_list.d*) lists all tracers needed in the simulation. Names and molecular weights are listed, as well as some diagnostic flags *that are not yet in use*.

The list is divided into two parts: the first lists the transported and the second lists the non-transported species. The total listed numbers of transported and non-transported species must match `NPAR` and `NOTRPAR` in *cmn_size.F90*.

When read into the model, the tracer names are found in the variables `TNAME` for transported species and `XTNAME` for non-transported species.

There may be a tracer list available for your choices, and they are located in the directory *tables*. You may have to make your own tracer list, depending on which applications you include.

It can be mentioned that eventually, the non-transported array should be removed, but this is left for future work.

Where is the tracer list specified?

The path and file name of the tracer list is specified in the input file *LxxCTM.inp*.

2.7.5 Emissions list – *Ltracer_emis_xxx.inp*

This file contains all emission information needed for the Oslo CTM3 to run; information on forest fires, lightning, 2D and 3D monthly emissions. The files are located in the directory *tables*. You may want to build your own list; just save it under a different name. There are files for different main inventories, such as CEDS, ECLIPSE, RETRO and Lamarque, listed in the subdirectory *EMIS-SION_LISTS*.

Important 1:

You should keep good track of the emission inputs you use in different model runs; they are important to be able to reproduce the simulations. For simplicity, the whole list is printed to standard out, before reading the file again and doing the actual read-in of emission datasets.

Important 2:

There is no default/preferred emission dataset yet, so you have to ask the experienced users about which you should use. There are several datasets for anthropogenic emissions, but fewer for natural emissions. Natural emissions will often have to be taken from several datasets.

Important 3:

If you want to include CH₄ emissions instead of using the standard fixed surface concentrations, you have to do some changes to the code and input files. To do this correctly, you **must** read Section 8.9.

Important 4:

If you want to build your own emission list, please read Section 8.3.

File names of emission files are listed along with scalings for each component which the file applies for. Also a few short term variations can be specified.

Note that the whole path for the emission files should be given in the emission list (*Ltracer_emis_XXX.inp*), so you don't have to link to the emission directory.

Emission data can usually be found in a directory available for all users. However, when you start using the Oslo CTM3, you should ask us where to find the data.

See Section 8 for further information on the emissions and the scaling possibilities.

2.7.6 Meteorological data

Traditionally, the Oslo CTM3 has been driven by meteorological data from the ECMWF Integrated Forecast System (IFS) model, in both 40-layer and 60-layer versions. In 2015, the ECMWF openIFS model was applied to generate new data locally at CICERO/UIO, covering a larger time period. This model is in principle similar to the IFS model.

You define which meteorological data to use in the file *LxxCTM.inp*. First you need to specify the dataset:

- **metTYPE**: Which type of data. **ECMWF_oIFSnc4** is openIFS data in netCDF4 format. **ECMWF_oIFS** is openIFS data in the UIO format. **ECMWF_oIFS** is the older IFS data in the UIO format.
- **metCYCLE**: The cycle number of the model used to generate meteorological data.
- **metREVN**: The revision number of the cycle version.

Note that the Oslo CTM3 is only set up for these datasets so far. When other data is used, a new read-in routine must be made, and then the cycle and revision numbers can still be used to define the model version.

Next you define the path where the meteorological data is located, **MET_ROOT**. The Oslo CTM3 will use **metTYPE**, **metCYCLE**, **metREVN** and **metTYPE** to make the full path of file names. This is carried out in the **INPUT** routine in file *initialize.f90*.

When you start using the Oslo CTM3, you should ask current users where to find the data.

Important

The openIFS meteorological data was updated from binary files to netCDF4 files late 2015. You can find more about the meteorological data and the data formats in Appendix H. If you need to run the old format, there is a separate read-in available, called *met-data_ecmwf_uioformat.f90*. The Oslo CTM3 should give you a hint about this if you specify an old **metTYPE**.

Important for older meteorology data

The old format will eventually be phased out. The new format has greater flexibility e.g. to read a field from the next time step and interpolate temporally between them. If that is included at some point, it will be difficult to use the binary files.

If you get very strange results in the first time steps, you may have chosen the wrong resolution data. Reading 60-layer data in a L40 model run, may not proceed past the end of the file. But a L60 run will try to read past the end of file of 40-layer data, and the model will crash.

2.7.7 Restart file

A restart file contains tracer distributions for all species in a simulation, as well as the moments for all the transported species. It allows you to continue a run without loss of tracer information, and while some aerosol packages can be started from zero, chemical components usually requires initial values.

There are several versions of read-in routines available. The standard read-in reads netCDF4 files, and is called **load_restart_file**, located in the file *stt_save_load.f90*. It is called from subroutine **SETUP_SPECIES** in the file *initialize.f90*, which is called from *pmain.f90*.

In the restart file, transported species have prefix **STT_**, and for these species there are also moments available, having prefixes **SUT_**, **SVT_**, **SWT_**, **SUU_**, **SVV_**, **SWW_**, **SUV_**, **SUW_**, **SVW_**. Non-transported species have prefix **XSTT_**.

The read-in will interpolate horizontally if the model resolution differs from the file resolution, but note that in such cases only two moments are used: **SWT** and **SWW_**.

A possibility for vertical interpolation should be included eventually.

The read-in assumes the restart file is called *restart.nc*, but note that it is possible to read several restart files. As long as the read in flag **MODE** is set correctly, only the uninitialised fields will then be set.

Complementary, there is a routine to save the restart files, called **save_restart_file**,

As a new user, you should regularly check that you actually use the restart file you think you use.

Traditionally you can also restart from a monthly average, but this needs more spinup. There is yet no routine for reading average netCDF files.

2.7.8 Other input data

There are some additional data you need for running the Oslo CTM3. The model reads these data from the directory *Input_CTM3*, so you need to link to that directory. On the Abel cluster this is located at */work/projects/cicero/ctm_input/Input_CTM3*, and the data consists of

- 2d-data for the stratospheric module (boundary condition data).

- Background aerosol surface area densities for the stratospheric module.
- CH₄ surface mixing ratios.
- Dry deposition values.

2d-data

Stratospheric chemistry includes a number of species which have long tropospheric lifetimes, and thus is set as fixed mixing ratios in the model levels closest to the surface. At the top of the model, i.e. upper stratosphere, the model lacks information on how much is transported upwards (into the mesosphere) and also on mixing ratios to be transported downwards (from the mesosphere).

Species having very long lifetimes and are destroyed in the mesosphere, they may build up in the stratosphere if the flux out is not considered. Likewise, if a component is produced in the mesosphere and transported downwards, it would not be included as a source for the stratosphere.

Traditionally, upper boundary conditions have been set for many species, mimicking this, while doing chemistry up to the next-to-uppermost layer (L_{PAR-1}).

These boundary conditions are taken from simulations done with the Oslo 2D model, and are just called the 2d-data. The data are read from the directory *Input_CTM3*, so you have to link this directory to where you run the model.

While such a method may hinder build-up of some species, it is for other species not an ideal solution.

- Firstly; the uppermost level of the 2D model is about 55 km, well below the L60 top level. The mixing ratios are therefore scaled to the L60 vertical grid using the uppermost mixing ratio gradient of the 2d-data (see Section 11.6 for more). Using 2d-data may perhaps be ok for L40, but not for L60.
- Secondly; depending on the tracer, it may effectively act as either a sink or a source. This may not be what was intended.
- A third obstacle is that upper boundary conditions must match the simulated year. Removing it will make modelling e.g. pre-industrial and future atmospheres easier.
- Finally, the Oslo 2D model can no longer be run because its input files are nowhere to be found. The 2D data are therefore not available for years after 2011.

One solution is to use e.g. WACCM to produce boundary conditions. Another, perhaps better, solution is to do chemistry all the way p to the model top, so that there is a fixed lid on top of the model. If a flux out or in is needed, it should be parameterised as a separate process. **I am currently trying to revise this (started January 2015).**

The 2d-data are read from original Oslo 2D files, so-called *sr-files*, and interpolation to model resolution is carried out on-line.

Stratospheric background aerosols

Background aerosol surface area density is important for the heterogeneous chemistry in the stratosphere. These data are also located in the directory *Input_CTM3/backaer_monthly/*.

These data were compiled by David Considine and Larry Thomason at NASA LaRC, based on SAGE II, SAGE I and SAM II satellites. Data was prepared by the approach of Thomason et al. (1997), and a description can be found in the *backaer_monthly/* directory.

The data are read from the original resolution and interpolated on-line to the model resolution.

Only year 1979 to 1999 are available, where 1979 is used for all years prior to 1979 and 1999 for all years after 1999.

Dry deposition

Dry deposition velocities are read from the file *dry-dep.ctm*, which is found in the *Input_CTM3* directory. A new dry deposition scheme is under way, and will replace this method or most species. See Section 7.2 for more.

2.7.9 Surface CH₄

Due to its long lifetime, CH₄ is usually fixed at the model surface. This is the default treatment in Oslo CTM3. The files containing this input data are located in the *Input_CTM3* directory. Surface volume mixing ratios were calculated in the project HYMN, where CH₄ emissions were included, and monthly averages for 2003, 2004 and 2005 are available for Oslo CTM3. Currently we use 2003 monthly values, however, these values should be scaled to match observed values for the year you are simulating. This can be done by a separate routine, scaling the HYMN 2003 dataset to marine global annual CH₄ observed by ESRL Global Monitoring Division (see Section A.2.5).

Important 1

For pre-industrial simulations, these will have to be scaled or updated.

To match these surface values, it is possible to also set the whole 3D tracer field from the HYMN results.

Important 2

As noted above, the fixed CH₄ field from HYMN can be scaled to observed values. If you use a CH₄ field from a different year, you can make a similar scaling routine (see Appendix A.2.5).

Not so important

Also available are RETRO surface values, as zonal means for different years.

CH₄ emissions

The Oslo CTM3 can also be run with CH₄ surface emissions. Currently the possible set-up is a combination of anthropogenic emissions and natural emissions and soil uptake provided by Bousquet (project GAME). If you want to include CH₄ emissions, you **must** read Section 8.9.

2.7.10 Transport options

Transport is explained in Section 6, however, there are two things worth mentioning before you start.

In the input file (*LxxCTM.inp*), you specify the duration of the operator split time step, i.e. the duration of each process. Default is `NROPSM=3`, which means 60 minutes when there are 8 meteorological time steps during the day (this is default in Oslo CTM3). This is not the time step used in the transport routine; this is further explained in Section 6. The operator split time step is the duration of each process before the next is started.

It is possible to run the Oslo CTM3 with as short operator split time step as wanted. Halving the value to `NROPSM=6` will improve the polar vortex gradients, and should be used when studying the polar stratosphere (Søvde et al., 2012).

In addition, it is possible to use a more accurate treatment of the polar cap transport. The improved transport improves cross-polar gradients and should also be considered for polar stratosphere studies. How to implement the more accurate transport is explained in the horizontal transport section in *pmain*.

2.8 Compiling

When the *Makefile* is set up, it can be compiled e.g. using *gmake*. Just type *gmake* and hit enter. Note that parallel compiling (e.g. *gmake -j8*) is faster.

When you change global parameters you need to re-compile the whole program, it is wise to first clean up the object files:

```
gmake clean
```

This cleans all the files generated by *gmake* during a compilation.

You can also check the contents of *Makefile* by *gmake check*.

2.9 Running the model

You start the model by typing

```
./osloctm3 < LxxCTM.inp
```

where *Lxx* is the vertical resolution you compiled with (including possible info on how layers are collapsed). Usually, Oslo CTM3 uses *L60CTM.inp*. You use the same input file for all horizontal resolutions. Horizontal resolution is set in *Makefile*.

Oslo CTM3 is parallelized using OpenMP (see Section 4.3), and for most machines you need to specify the number of threads in an environment variable (`OMP_NUM_THREADS`). This can be handled automatically by a job script, or you may have to specify yourself. You can e.g. use 16 CPUs by running:

```
OMP_NUM_THREADS=16 ./osloctm3 < LxxCTM.inp
```

Note that this will print to screen. To print to a log file, use

```
OMP_NUM_THREADS=16 ./osloctm3 < LxxCTM.inp > results.log
```

Add the standard `&` at the end to make the program run in the background.

2.9.1 Model crashes

As a new user you will probably experience that the model crashes when you try to run the model for the first time.

A couple of diagnostics require certain tracers to be included, and if they are not, the model will crash. These are:

- `satprofs_master`
- `vprofs_master`
- `caribic2_master`
- `trocciXXX_master`

To solve this, you may either change the list of tracers in their corresponding files, or you may comment out the calls to the routines. The latter is done in the routine `nops_diag` in *diagnostics_general.f90*.

Note that the calls are by default commented out, so you have to put them back if you need them.

You should also check out the Appendix I for trouble shooting.

2.10 Publishing & documenting

Not only should we publish research in peer-reviewed journals, we should also document changes in the Oslo CTM3, at least if the changes are introduced to the repository.

2.10.1 Publishing in journals

When you publish results from the Oslo CTM3, please let the Oslo CTM3 users know of it!

I have included a list of papers in Appendix K.

Contact info is found in Appendix L.

2.10.2 Documenting changes

If you upgrade the Oslo CTM3 (other than small bug fixes) please write up a description document, including the main effects.

3 Source code introduction

This section provides a short description of the model source code, which is mainly written in Fortran90 with file extension *-.f90*. However, there are a few files written in fixed form with extension *-.f*. The latter comprise the most important transport files inherited from UCI, and

were not converted to make possible future updates from UCI easier.

Oslo CTM3 is free from common blocks. All variables are defined in modules.

Model source code files are generally divided into core files and files needed for Oslo chemistry and aerosols modules. The Oslo files are located in the directory *OSLO*.

Model parameters and variables are found in the *cmn*-files, see Section 3.1.2.

Note that several modules also contain their own global variables.

See Section 4 for program structure and Section 5 for programming guidelines.

3.1 The core source

The model core consists of the files (routines, variables, parameters) necessary to run the model with transport only, e.g. meteorological variables and tracer distribution variables. The core source is located in the main directory, and are based on the files inherited from UCI.

The global variable *cmn*-files are placed in several files, described in Section 3.1.2.

Essential to the model is the tracer distribution of the transported species, named *STT*, which is a 4D array of model grid size (see Section 2.4 for grid description) times the number of *transported* components (*NPAR*). See Section 3.2 for how to handle the non-transported species.

Inside the parallelisation loops, the tracer field (*STT*) is moved into local arrays (*BTT*), which have a different structure. We will call this a *B-array* (or private array), and its structure will be explained in Section 4.3.

The second order moments scheme also transports the first and second order moments, i.e. 9 moments for each of the transported species. These moments are named *SUT*, *SVT*, *SWT*, *SUU*, *SVU*, *SWU*, *SUV*, *SUW*, and *SVW*, and are described in Section 6. Also the moments are transformed into B-arrays in the parallel region.

3.1.1 The parameter files

Central to the model core is the parameter file *cmn_size.F90*, which sets the model resolution (i.e. array sizes) through the parameters *IPAR*, *JPAR*, *LPAR*, *NPAR*, etc.

This file uses the *Makefile* tokens to include chunks of code defined by the C-code (such as *#ifdef*). All parameters are set automatically when compiling with well known user choices in *Makefile*.

Among the parameters are also logical switches for each of the chemistry or aerosol modules, such as

- *LOSLOCTROP*: Use Oslo tropospheric module.
- *LOSLOCSTRAT*: Use Oslo stratospheric module.
- *LSULPHUR*: Use Oslo sulphur module.
- *LBCOC*: Use BCOC module.

Makefile was described in Section 2.7.1.

3.1.2 Global variable files

The global variable files (common files) are:

- *cmn_precision.f90*: Defines precision parameters.
- *cmn_size.F90*: Parameters for grid sizes and also logical parameters needed for the run.
- *cmn_ctm.f90*: Transport variables and more.
- *cmn_chem.f90*: Emission variables and other variables related to chemistry.
- *cmn_fjx.f90*: Variables for fast-JX (photochemistry).
- *cmn_met.f90*: Meteorological variables.
- *cmn_sfc.f90*: Surface (2-dimensional) variables.
- *cmn_diag.f90*: Diagnostic variables.
- *cmn_parameters.f90*: Parameters.
- *OSLO/cmn_oslo.f90*: Variables for Oslo chemistry and aerosols.

3.1.3 Main program

The main program is located in *pmain.f90*. It is described in Section 4.

3.1.4 Core diagnostics

The main diagnostics are baked into the model core, and also have a few B-arrays. Such B-arrays bring their diagnostics back to the upper level, where they usually are put out every operator split time step, or e.g. accumulated for averaged values. The diagnostics will be described further in Section 21.

3.2 The Oslo core source

The Oslo core comprises the files and variables necessary to run the model with Oslo packages. The files are located in the directory *OSLO*.

Variables are generally located inside modules or in *cmn_oslo.f90*, whereas the subroutines are mostly located in modules.

3.2.1 Important variables

In chemistry, each component has a chemical id, and these ids must be mapped to transport number. This is done in the variable *trsp_idx* maps the transported species (chemical IDs) into their transport number – i.e. into their place in the *STT* array. In the same way *Xtrsp_idx* maps the non-transported species into their place in the non-transported tracer array *XSTT*. The sizes of the mapping arrays are set by the maximum number of chemical IDs (*TRACER_ID_MAX* in *cmn_size.F90*).

Similarly, two other index arrays map the other way; *chem_idx* (size *NPAR*) and *Xchem_idx* (size *NOTRPAR*), respectively.

These can be found in the files *cmn_ctm.f90* and *cmn_oslo.f90*, respectively.

XSTT is located in *cmn_oslo.f90*.

Note that if you have no non-transported species, the array size will of e.g. *Xchem_idx* will be zero. This means that before trying to access this array, you need to check if *NOTRPAR* is greater than zero, otherwise the program may stop.

To diagnose the non-transported species, a 3D average field is also defined (*XSTTAVG*). This average field follows the Oslo CTM3 core average treatment. Note that these arrays are reverse-indexed (*IPAR*, *NOTRPAR*, *IPAR*, *JPAR*) to reduce striding, since they are only accessed in the IJ-blocks. They keep this structure when written to the restart file and to average files.

Important

The use of non-transported species should be out-phased and replaced by some steady-state considerations, but this will be left for later.

3.2.2 Application variables

Variables that are only used by a specific application are in general defined in their respective modules or files.

3.2.3 Dummies

To be able to turn off an application, most applications have some dummy routines, located in *OSLO/DUMMIES*. See Section 4.1.4 for more.

4 Program structure

To get an overview of how the Oslo CTM3 works and how it is structured, it is best to look into the main driver *pmain* (*pmain.f90*).

4.1 Main structure – *pmain.f90*

The main program (*pmain.f90*) controls the main loops and calls to do the calculations. Its general structure is outlined in Table 1, with the important loop variables *NDAY*, *NMET*, *NOPS*, and *NSUB*. They are all defined in *pmain*, and are thus not global variables.

4.1.1 Main loops

NDAY is the day counter, looping through each day (from *NDAYI* to *NDAYE-1*, see Section 2.7.3). These variables are therefore defined in *pmain* (not global). Things that need to be done on daily basis will be placed in this loop. Daily diagnostics, however, should be placed at the end of the day.

NMET is the meteorological time step. For ECMWF IFS data, the meteorological data is stored 8 times per day

Table 1: The general structure of the main program.

```

<initialize model>
!// MAIN LOOP
do NDAY = NDAYI,NDAYE-1

    <do daily stuff>

    !// METEOROLOGICAL LOOP
    do NMET = 1,NRMETD

        <update meteorology etc>

        !// OPERATOR SPLIT LOOP
        do NOPS = 1,NROPSM

            !// SUB LOOP
            do NSUB = 1, LCM
                !// do master calls
                <chemistry>
                <transport>
                <diagnostics>
            end do

            <diagnostics after every NOPS>
        end do

        <diagnostics after every NMET>
    end do

    <daily diagnostics>
end do

```

(00UTC, 03UTC, ...). The number of meteorological time steps is set by the *NRMETD* parameter defined in *cmn_size.F90*. It should be noted that some ERA-40 data are also available. These are also ECMWF data, but given 4 times per day. The Oslo CTM3 is not set up to use them, however, if you want to use ERA-40, you should change the number of meteorological time steps *NRMETD*. A less optimal method is to read the data every second *NMET* and not changing *NRMETD*. I would not recommend this, but if you insist, remember in read-in to change the time step used for scaling the accumulated data.

NOPS is the operator splitting time step, with a duration of *DTOPS*. Operator splitting means that the operations are done in sequence, with a certain time step. There number of such sequences per meteorological time step is given by *NROPSM*. For a short enough time step the operations should be close to reality, and the solution should converge when further shortening the time step. Keep in mind that the order of the processes may be important. Note that the meteorology is kept constant through the meteorological step, no matter how many operator split time steps are used.

Within each *NOPS*, there is a sub-stepping loop where chemistry and transport are done asynchronously if their time steps differ. This will be explained next.

Table 2: Examples of sub-stepping (NSUB) with uneven time steps.

Example 1: NADV=1 and NRCHEM=4, with NLCM=4:

| Step | What is done | Time durations |
|------|--------------|----------------|
| 1 | CHEM ADV | 15min / 60min |
| 2 | CHEM | 15min |
| 3 | CHEM | 15min |
| 4 | CHEM | 15min |
| 1 | CHEM ADV | etc... |

Example 2: NADV=3 and NRCHEM=4, with NLCM=12:

| Step | What is done | Time durations |
|------|--------------|----------------|
| 1 | CHEM ADV | 15min / 20min |
| 2 | | |
| 3 | | |
| 4 | CHEM | 15min |
| 5 | ADV | 20min |
| 6 | | |
| 7 | CHEM | 15min |
| 8 | | |
| 9 | ADV | 20min |
| 10 | CHEM | 15min |
| 11 | | |
| 12 | | |
| 1 | CHEM ADV | etc... |

4.1.2 Sub-stepping loop

During one operator split loop (for each NOPS) advection is done NADV times (calculated based on numerical stability), while chemistry and boundary layer mixing are done NRCHEM times. NRCHEM is set by the user in *LxxCTM.inp*, with a default value of 1. See section 4.1.3 for more on this variable. The corresponding time steps are $DTADV = DTOPS/NADV$ and $DTCHM = DTOPS/NRCHEM$, respectively.

Operations are in general done in sequence (operator splitting), but when time steps DTADV and DTCHM differ the result is an asynchronous stepping. The sequence of operations is solved by looping through the least common multiple (NLCM) and do advection and chemistry accordingly. This is done by NSUB in Table 1. Figuratively, this can be shown by some examples, given in Table 2.

It follows from these examples, that when NADV and NRCHEM are larger than 1, the operations are done more frequently than once per NOPS, and should therefore be closer to reality.

Note that the processes in general do not start at the same hours and minutes, but are asynchronous: Example 2 in Table 2 shows this. The processes are carried out using different time steps ($DTADV = DTOPS/3$ vs $DTCHM = DTOPS/4$), so that at NSUB=5, chemistry has already been calculated (4-6) when advection is calculated (5-9)

Both chemistry and advection is done in the first NSUB, so that in Example 1, chemistry is done for 60 minutes consecutively (4 times of 15 min), starting at step 2, before the next advection.

4.1.3 Internal chemistry loop

Considerable CPU time is used to go in and out of the B-array parallel region. The reason for this is that advection needs two types of parallel coding (IJ-block, Section 4.3.2 and layer parallelisation, Section 4.3.3). If the processes that only need IJ-block parallelisation (e.g. chemistry) is carried out more often, the time spent on moving in and out of the B-arrays will increase.

It is therefore preferable to set NRCHEM as low as possible. However, the number of operator splits is usually 3, which for NRCHEM=1 will give a time step of one hour for each of the processes (emissions, boundary layer mixing, chemistry and deposition). This may be a little too long in the boundary layer, where mixing is relatively fast.

Traditionally, the Oslo CTM2 solved this by looping boundary layer mixing and chemistry with a time step of 15 min. We adopt this in Oslo CTM3, introducing an internal loop over emissions, boundary layer mixing, chemistry and deposition in pmain. The looping is carried out CHMCYCLES times per NOPS; for NRCHEM=1, CHMCYCLES=4, for NRCHEM=2, CHMCYCLES=2 and otherwise CHMCYCLES=1.

Note that the chemical section (emissions, boundary layer mixing, chemistry and deposition) is still calculated for one NRCHEM before advection is calculated.

Future update

I think it would be a good idea to let NRCHEM change according to NADV; in T42 resolution, we often have NADV=1, but also encounter larger values, especially in higher resolutions. The code should be modified to be able to account for this.

4.1.4 Important notes

Do not mess with pmain.f90!

pmain.f90 is supposed to be very short and easy to grasp. As few as possible calls should be made from pmain, and the calls should preferably be to master routines (e.g. diagnostics or chemistry).

Keep the model clean of C-code!

If you do not know what C-code may do in the Fortran code, all is well. Or you can check Section 4.2. C-code should not be necessary to include or exclude parts of code. It makes the code very difficult to read, at least for large chunks of code. Even if one programmer introduces a new small chunk of C-code, experience has shown that this practice will grow. If you insist on using them in your subroutines or modules, keep the existing code free of C-code.

In the model core, there is only one file containing C-code, and that is *cmn_size.F90*, which is the basis for *Makefile* to generate important parameters. (In the Oslo core, the DUST code also contain some C-code.)

Instead of C-code, dummy routines should be used in the model code. The time spent on calling a routine which in worst case does nothing (see Section 4.2), is very minute compared to spending time on a messy program code. The compiler will in most cases remove the call to an empty routine, removing calling overhead by inlining the

code (which is empty). See the files in *OSLO/DUMMIES* for dummy examples.

4.2 The C-code preprocessing system

The C-code preprocessing system is a way to include or exclude chunks of code from being compiled. The pre-processor will look for specified *tokens*, e.g. `DO_THIS`. In the preprocessing the code located between the statement `#ifdef DO_THIS` and `#endif` will then be compiled. The C-compiler will make a temporary file which will be compiled by the Fortran compiler.

Files containing such C-code will typically only be located in files with extensions `-.F` or `-.F90`.

We will avoid C-code in the model, except in *cmn_size.F90*, where the tokens are coupled to settings in *Makefile*.

4.3 Parallelisation of the Oslo CTM3

The Oslo CTM3 is parallelized using OpenMP. The general parallelisation is done in *pmain.f90* and is carried out in two different ways, which will be described in Section 4.3.2 and 4.3.3:

1. Over IJ-blocks: Applies for chemistry, boundary layer mixing, convection and vertical advection.
2. Over vertical layers: Horizontal advection only.

In addition some other routines outside parallel regions are parallelized, e.g. emission interpolation.

4.3.1 OpenMP

The OpenMP code can easily be located by the `!$OMP` at the beginning of a line of code. It is followed by different specifications, e.g. `!$OMP PARALLEL`. One of the important issues is to understand the meaning of `PRIVATE` variables; they are private to each thread/CPU. `SHARED` variables are shared. By default, as a safety measure, you have to define *all* variables inside a parallel region (not necessary for parameters, which cannot be changed).

If you want to learn more about OpenMP, see <http://openmp.org/>. Also, the Fortran company provides a tutorial on their web page <http://www.fortran.com/>.

4.3.2 Parallel IJ-blocks (MP-blocks)

Most processes are either independent of neighboring grid boxes, or they depend on the grid box above or below. In the Oslo CTM3 these processes are treated column-wise, and the columns are grouped together in blocks of a certain horizontal extent.

In this way the model domain ($\text{IPAR} \times \text{JPAR} \times \text{LPAR}$) is split into blocks (so-called IJ-blocks or MP-blocks) beneficial for parallel work: IPAR is divided into MPIPAR sections, and JPAR into MPJPAR sections, while LPAR is unchanged. This creates $\text{MPIPAR} \times \text{MPJPAR}$ blocks of size

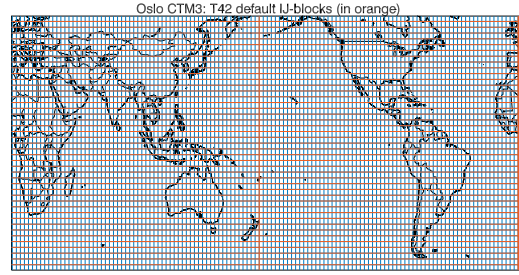


Figure 1: Default IJ-block structure for T42 horizontal resolution, where one block covers half the zonal direction and one latitude band.

(LPAR , IDBLK , JDBLK) which are fed into the parallelisation ($\text{IDBLK} = \text{IPAR} / \text{MPIPAR}$ and $\text{JDBLK} = \text{JPAR} / \text{MPJPAR}$).

Useful related parameters are $\text{IDGRD} = \text{IPARW} / \text{IPAR}$ and $\text{JDGRD} = \text{JPARW} / \text{JPAR}$, giving the number of grid boxes combined in each direction. Total number of grid boxes combined is NDGRD .

For the IJ-blocks, the transported 4D arrays (STT , and moments) are split into temporary private arrays (B -arrays) available for each processor, where the spatial size is (LPAR , IDBLK , JDBLK). The index order has been “reversed” (i.e. the LPAR first instead of last) to minimize striding when working vertically. See Section 5.11 for more on striding.

Due to the IJ-block array structure, the loops will produce less striding for long zonal blocks. Depending on the resolution, the choice of MPIPAR and MPJPAR must be tested to find which is faster. For T42 and 2×2 combined T159 horizontal resolutions the default is $\text{MPIPAR} = 2$ and $\text{MPJPAR} = \text{JPAR}$. The IJ-blocks are constructed to cover half of the zonal direction ($1 : \text{IPAR} / 2$), and one latitude band, as shown in Figure 1. It may be that other configurations are better when transporting few tracers. For other resolutions there are other block sizes (defined in *cmn_size.F90*). A more thorough discussion on the IJ-block sizes is included in Section 4.3.6.

In *pmain.f90*, the parallel index M loops through the number of IJ-blocks, and is passed on to subroutines where it is usually named MP . The global indices are accessible by using the variables MPBLKIB , MPBLKIE , MPBLKJB and MPBLKJE (all of size MPBLK). Their names MPBLKIB and MPBLKIE are somewhat self-explaining; the first contains the zonal beginning point of all IJ-blocks (i.e. the global zonal indices), while the latter contains the end points. Similarly, MPBLKJB and MPBLKJE are the starting and end points in the meridional direction. For a given IJ-block (which have parallel index MP), the first global zonal index therefore is given by $\text{MPBLKIB}(\text{MP})$ and ends at $\text{MPBLKIE}(\text{MP})$, while the first global meridional index is given by $\text{MPBLKJB}(\text{MP})$ and ends at $\text{MPBLKJE}(\text{MP})$.

A typical IJ-block loop is outlined in Table 3, and you should understand how it works and why the reverse-ordered B -arrays provide less striding (see Section 5.11 for more on striding). For global indices I, J the local/private indices for IJ-block number MP are given by $\text{II} = \text{I} - \text{MPBLKIB}(\text{MP}) + 1$ and $\text{JJ} = \text{J} - \text{MPBLKJB}(\text{MP}) + 1$.

Table 3: Looping through an IJ-block and accessing global and private variables, for component N.

```

!// Loop over latitudes in IJ-block
do J = MPBLKJB(MP),MPBLKJE(MP)
!// IJ-block index JJ
JJ = J - MPBLKJB(MP) + 1

!// Loop over longitudes
do I = MPBLKIB(MP),MPBLKIE(MP)
!// IJ-block index II
II = I - MPBLKIB(MP) + 1

!// Corresponding local/global
!// indices
BTT(L,N,II,JJ) = STT(I,J,L,N)

enddo
enddo

```

A mapping from global indices I,J to IJ-block number and local indices can be found in the variable `all_mp_indices`:

```
(II,JJ,MP) = all_mp_indices(1:3,I,J)
```

4.3.3 Parallel layers

Horizontal advection, i.e. transport between neighboring grid boxes, have no need for information about boxes above or below. Hence, this process carried out layer by layer, and a processor calculates transport of all tracers for one layer, before being assigned (by OpenMP) a new layer to transport.

It is also possible to do the transport component by component, so that each processor work on each species, transporting them layer by layer. Although this was done in Oslo CTM2, it is not done now. The experience of the UCI group was that looping over layers is faster. *Note also that studies with few tracers would limit effective use of the number of CPUs, if parallelisation is done over components.*

4.3.4 OpenMP and advection

The important consequences of the advection treatment (Section 4.3.2 and 4.3.3) is that advection works both in IJ-block and layers and therefore need to go in and out of IJ-blocks for each transported time step. It means that increasing the number of operator split steps, also increases the time spent shuffling data in and out of B-arrays; transport may be better resolved, but it will be slightly more time consuming.

4.3.5 Writing parallelized code

When you write a new module, be sure to parallelize it! For most processes or applications, it would be wise to use the IJ-block structure, and therefore assign global arrays in reverse order (L_{PAR}, I_{PAR}, J_{PAR}), or even better

Table 4: Computational efficiency when increasing the number of CPUs for T42L60 resolution. Timings are given in wall clock hours, for pure transport of 32 and 64 tracers, T42L60 resolution, meteorological data for January 2005

| | T42L60_32 | T42L60_64 |
|---------|-----------|-----------|
| 4 CPUs | 1.72 | – |
| 8 CPUs | 0.92 | 1.95 |
| 16 CPUs | 0.57 | 1.08 |
| 32 CPUs | 0.46 | 0.67 |
| 8:4 | 0.53 | – |
| 16:8 | 0.62 | 0.55 |
| 32:16 | 0.81 | 0.62 |

by blocks (L_{PAR}, I_{DBLK}, J_{DBLK}, MPBLK).

If your application works in the horizontal (this is less likely), parallelisation should be layerwise, and global arrays should *not* be reverse order but have the usual structure (I_{PAR}, J_{PAR}, L_{PAR}).

Example: If you use 4 processes and your unparallelized application uses 5 seconds per time step (assuming one hour), it will contribute with ~ 12 hours of computing time when simulating one year. Effectively parallelized, you could possibly divide this by the numbers of processors, so that in using 4 CPUs you save 9 hours of real computing time.

4.3.6 How many CPUs and IJ-blocks?

The more done in parallel, the more efficient and faster will the program be. The Oslo CTM3 is better parallelized than the Oslo CTM2, however, there are a few things you should be aware of when it comes to the choice of CPU numbers and how it relates to the number of IJ-blocks.

The number of IJ-blocks (set up in `cmn_size.F90` should be a multiple of the number of CPUs, since the amount of work done in a column should be approximately the same for all columns. It's more difficult to do such a choice for the horizontal transport, since the amount of work done differ from layer to layer (shorter time step for larger wind speeds). However, the time spent in horizontal transport is relatively small, so a good choice for the number of CPUs will be a multiple of the number of IJ-blocks. As will be explained, the number of IJ-blocks should be at least twice as large as the number of CPUs.

Timing tests of pure transport are included in Table 4, showing that transporting 32 tracers on 8 CPUs and switching to 16 CPUs saves $\sim 40\%$ time, while switching from 16 to 32 only saves 20%. However, transporting 64 tracers and switching from 16 to 32 CPUs also saves about 40%. Hence, the number of IJ-blocks should be at least twice as large as the number of CPUs.

The number of IJ-blocks and how they are defined also affect how efficient the parallel code will be. For the setting MP_IPAR=1 and MP_JPAR=JPAR/2, each block will cover the whole zonal direction (1: I_{PAR}) and two latitude bands. Table 5 shows a few tests carried out for meteorolgy data of 1 January 2005, comparing CPU timings for different

Table 5: Computational efficiency for different choices of IJ-block sizes, for 64 tracers in T42L60 resolution. Timings are for one day of transport (1 January 2005), given in wall clock seconds.

| Pure transport (average for 4 tests per case). | | |
|--|--------|--------|
| MPIPAR/MPJP | 16 CPU | 32 CPU |
| 1/16 | 120.8 | 112.0 |
| 1/32 | 122.0 | 71.4 |
| 2/16 | 119.6 | 72.5 |
| 1/64 | 116.7 | 69.6 |
| 2/32 | 115.0 | 69.3 |
| 2/64 | 110.8 | 68.0 |
| Full chemistry (average for 3 tests per case). | | |
| MPIPAR/MPJP | 16 CPU | 32 CPU |
| 1/32 | 256.3 | 151.7 |
| 2/32 | 245.9 | 144.8 |
| 2/64 | 245.0 | 145.0 |

IJ-block sizes.

From Table 4, we found that the number of blocks should be at least twice the number of CPUs. Additional runs have been carried out to put further light on this.

It should be easily recognised that the number of IJ-blocks should be at least as large as the number of CPUs. This is expected because the program is parallelized over IJ-blocks. 16 IJ-blocks on 32 CPUs is only slightly faster than on 16 CPUs because horizontal transport is parallelized over 60 model layers, and thus is where the main improvement is.

Due to e.g. read access limits, the timings may vary slightly. Therefore each test was done 4 times, and the values presented in Table 5 are averages. It seems that MPIPAR=2 and MPJP=JP is fastest for T42L60 transport, followed closely by MPIPAR=2 and MPJP=JP/2.

One-day tests with full tropospheric and stratospheric chemistry show that on 16 CPUs, MPIPAR=2 and MPJP=JP saves about 10 s per day, compared to MPIPAR=1 and MPJP=JP/2. Note that 10 s per day amounts to ~1 hour of computing time for one year. For T42L60, the configuration MPIPAR=2 and MPJP=JP/2 seems to be almost as fast as MPIPAR=2 and MPJP=JP on 16 CPUs, and slightly faster on 32 CPUs. As the default IJ-block size for T42 we set MPIPAR=2 and MPJP=JP.

Using a different date, where the meteorological conditions impose a shorter time step (10 Jan in this case), indicates that IJ-blocks spanning more than 2 meridional boxes, e.g. MPIPAR=2 and MPJP=JP/4, seem to make transport slower.

For higher resolutions, we keep the IJ-block of size 1:IPAR and one latitudinal band. On 32 CPUs, T159L60 transport is faster for MPIPAR=1 and MPJP=JP, while that was not the case for T42L60. This is due to memory and striding issues.

The main lesson is: Keep the number of IJ-blocks as close to a multiple of CPUs as possible. If not, CPUs may be partially idle during computation; e.g. when using 80 IJ-blocks for T159L60 on 32 CPUs, half of the CPUs will

on average do 3 IJ-blocks, while the rest does 2. Vertical transport may change this slightly if time steps differ greatly in different IJ-blocks. However, a multiple (greater than 1–2) of the number of CPUs seems to be the best choice.

On 16 CPUs it may be that 80 IJ-blocks works well for T159L60, being a multiple of 5. If you want to use 64 CPUs, you should use MPIPAR=2 and MPJP=JP, i.e. 320 IJ-blocks. Keep in mind that a 32 CPU machine set up with hyperthreading often is referred to as having 64 CPUs. This is not true, and the Oslo CTM3 will most probably run as fast as using 32 CPUs (or sometimes even slower).

In essence, when using other resolutions, you should check different choices of IJ-blocks to find which is faster.

If you plan to use only one processor (serial run), you should still use several IJ-blocks! E.g. one global IJ-block will be large and not very efficient, since the whole global arrays will have to be re-arranged. Remember also that the efficiency is greatly reduced in a serial run, since the re-arranging of the structure is time consuming *and carried out by one processor only*.

4.4 Module based programming

The model code has evolved from being partially Fortran90 to being fully Fortran90 in 2015. Common blocks are no longer used, as they are marked obsolete by the Fortran company.

When you add new packages, you should program them as modules. It is more flexible, and allows combining fixed format code with free format code. Another advantage is that you can define which parts of a module you want to access. You access the whole module with

```
use <module>
```

where <module> is the name of the module. This statement must be placed before the `implicit none` statement.

However, you get a better code, which is easier to read and search or debug, when you specify the variables and subroutines to use:

```
use <module>, only: <variables, subroutines>
```

where <variables, subroutines> is the list of needed variables and/or subroutines, separated by commas.

If you include a module A, which again includes a module B, you have indirectly access to all variables and routines in B. By using the `only` statement, this can be restricted.

For programming guidelines on how to make your subroutines optimal for the Oslo CTM3, see Section 5.

5 Programming guidelines

Think structure! If you do not understand the structure of the model (Section 4), you will probably end up with a very messy and inefficient code.

A messy code may solve your problem, but should *never* be added to the Oslo CTM3 repository!

5.1 Comment your code!

Comment your code! Others should understand your code (and yourself included after putting the code away for a while). If you do simplifications or approximations, include a comment about why.

Comment so that a newbeginner should understand quickly. Never include comments that are not understandable, such as “be careful”.

You should at least describe the following:

- Each module at the top of the file; its purpose and what it contains.
- Each subroutine, its purpose and variables, including the units of variables.
- All calculations. Include exact references if possible; if no reference is available, write why you do what you do. Write a description that can be included in this manual at a later stage.

5.2 Change existing code?

You should try to stay away from the existing core code except for making master calls at the top level (pmain) or in master routines themselves. If you think you need to do changes (especially big changes) in the existing code, check with the experienced programmers to find out if there may be better ways.

5.3 Accessing variables in Fortran90 free format

The Fortran90 free format is much easier to read than the fixed F77 style format, and is more elegant. E.g., there is no limit on the number of characters used on each line.

You can access variables from other modules in this way:

```
use cmn_size, only: IPAR
```

5.4 Adding a new subroutine

When you add a new subroutine it should be included in a module. Global variables or parameters should also be specified in this module, or possibly in common modules.

Still, there may be some very very few occasions, where it may be necessary to add arrays to the core or the existing chemistry files, but it should generally be avoided.

When adding a new file, you need to include it in *Makefile*. How to do this is explained in Appendix C.4.

5.5 Adding new components

When you add components, you need to make sure to change the number of tracers in *cmn_size.F90*, so that *Makefile* selects the right numbers in compiling. Also make sure the tracer list (*tracer_list.d*) has the correct tracer numbers, names and molecular masses.

The default length of tracer names (TMASS and XTMASS) is 10, set by TNAMELEN in *cmn_size.F90*. If you need longer names, you have to modify TNAMELEN.

Scavenging parameters are located in the file *scavenging_wet.dat* and *scavenging_dry.dat*.

5.6 Efficient code

Think parallel! Whether you add processes or diagnostics, the work should be done in parallel regions.

Diagnostics may be a little tricky, since they often require access to the global arrays. In this case, try to keep the arrays small, and do calculations in the parallel regions. The goal is to do as little as possible outside of the parallel regions (see Section 4.3.5).

If you need to convert a few tracers to another unit, you should only convert the ones you need. See Section 5.7 for more information on this.

5.7 Unit conversion

The tracer arrays are given in mass (kg) per grid box, and when you need another unit you should create a temporary array and convert it on the fly, avoiding routines converting the whole tracer array.

All tracers are, however, converted before chemistry, and put into the local array ZC_LOCAL (also stratospheric components before doing tropospheric chemistry). There is probably not much/anything to gain by only converting the tropospheric components for tropospheric chemistry and vice versa for stratospheric chemistry, but it may be revised at a later stage. However, only the tropospheric column is converted before tropospheric chemistry (1:LMTROP(I,J)), and only the stratospheric column before stratospheric chemistry (LMTROP(I,J)+1:LPAR).

The conversion routines are located in *utilities_oslo.f90*. Next follows descriptions of the conversions, you will probably need them.

5.7.1 Mass to concentration

The unit of concentration is molec/cm³. Conversion from mass (m_t) to concentration (c_t) involves the molecular mass (unit g/mol) and volume (m³). The conversion is done by

$$c_t = m_t \frac{10^{-3} N_A}{M_t V} \quad (5)$$

where N_A is the Avogadro's number (6.022149 × 10²³ molec/mol), M_t is the molecular mass (or weight) of the tracer (g/mol), and V is the grid box volume (m³).

The factor 10^{-3} is a combination of converting m_t from kg to g and volume from m^3 to cm^3 .

Converting the other way;

$$m_t = c_t \frac{10^3 M_t V}{N_A} \quad (6)$$

M_t is given in `TMASS` for transported species and `XTMASS` for non-transported species. Remember that they are indexed after transported and non-transported numbers, not tracer IDs, so to get the correct molecular masses you need the index arrays `trsp_idx` and/or `Xtrsp_idx`.

5.7.2 Mass to mixing ratio

By the term mixing ratio, the atmospheric chemistry community often mean mole/number mixing ratio, which as I will show is the same as volume mixing ratio for an ideal gas. In the aerosol field, however, mass mixing ratio is more common.

Mass mixing ratio (mmr) unit is kg/kg, i.e. mass of tracer (m_t) divided by the mass of air (m_a). On the other hand, mole (or number) mixing ratio is the number of tracer molecules (n_t) divided by molecules of air (n_a). For an ideal gas, concentration is $c_t = n_t N_A / V$, and $c_a = n_a N_A / V$, so the mixing ratio by volume is c_t / c_a .

For a specific tracer, the relationship between mole (n_t) and mass (m_t) is:

$$n_t = \frac{m_t}{M_t} \quad (7)$$

Thus, the conversion from mmr to vmr only involves the tracer mass (m_t), air mass (m_a) and the molecular weights of the tracer (M_t) and air (M_a):

$$\text{vmr} = \frac{n_t}{n_a} = \frac{\frac{m_t}{M_t}}{\frac{m_a}{M_a}} = \frac{m_t}{m_a} \frac{M_a}{M_t} \quad (8)$$

The number M_a / M_t is available as `TMASSMIX2MOLMIX` for transported species and `XTMASSMIX2MOLMIX` for non-transported species.

Note also that m_t / m_a is the mass mixing ratio *mmr*.

Converting back to mass:

$$m_t = \text{vmr} \times m_a \frac{M_t}{M_a} \quad (9)$$

M_t / M_a is available as the variable `TMOLMIX2MASSMIX` for transported species and `XTMOLMIX2MASSMIX` for non-transported species, so to convert to mass mixing ratio you multiply with `TMOLMIX2MASSMIX` (or `XTMOLMIX2MASSMIX`) and then multiply with the air mass.

5.7.3 vmr to mmr

The conversion from mass mixing ratio (mmr) to volume mixing ratio (vmr) is very short and easy. Given tracer mass (m_t), tracer moles (n_t), air mass (m_a), air moles (n_a) and the molecular weights of the tracer (M_t) and air (M_a):

$$\text{mmr} = \frac{m_t}{m_a} = \frac{n_t M_t}{n_a M_a}$$

$$= \text{vmr} \times \frac{M_t}{M_a} \quad (10)$$

In other words: multiply volume mixing ratio by `TMOLMIX2MASSMIX` (or `XTMOLMIX2MASSMIX` for non-transported tracers).

5.7.4 Concentration to mixing ratio

You should not need this conversion, but I include it in case you are interested. For an ideal gas the volume mixing ratio equals molecules of tracer divided by molecules of air, i.e. concentration of tracer divided by concentration of air:

$$\text{vmr} = \frac{c_t}{c_a} \quad (11)$$

c_a is the concentration of air - i.e. air density (mole/cm^3), while c_t is the tracer concentration. The air density is given as `AIRMOLEC_IJ`, a global field on IJ-block structure (`LPAR`, `IDBLK`, `JDBLK`, `MPBLK`) which is updated in the B-region at each meteorological time step.

Equation (11) can also be derived from Equation (6) and (8):

$$\begin{aligned} \text{vmr} &= c_t \frac{10^3 M_a V}{m_a N_A} \\ &= \frac{c_t}{c_a} \end{aligned} \quad (12)$$

Back to concentration:

$$\begin{aligned} c_t &= \text{vmr} \frac{10^{-3} m_a N_A}{M_a V} \\ &= \text{vmr} \times c_a \end{aligned} \quad (13)$$

5.8 Keep pmain clean

As noted in Section 4.1.4, you should not make large changes in *pmain.f90*. It is supposed to be very short and easy to grasp. Only simple master calls should be made from *pmain* (which is possible; write master routines!).

5.9 Precision of numbers

Variables should in general be defined as double precision, although there are some exceptions. The precision parameters are set in *cmn_precision.f90*, and you should follow the existing code. Do *not* use the old `real*8` method.

There are several definitions for precisions:

- `r8` is double precision.
- `r4` is single precision.
- `rMom` is the precision of the second order moments (standard is single precision).
- `rAvg` is the precision of average diagnostic arrays.
- `rTnd` is the precision of budget tendency arrays.

Most computers work faster on double precision than on single precision, so you should use double precision for floating point numbers. Only for very large arrays a gain can be achieved by using single precision, since it may reduce the number of cache misses. See Section 6.1 for an example of this.

Table 6: Correct traversing of an array in Fortran.

```

do J=1,JPART
  do I=1,IPART
    ARR(I,J) = ...
  enddo
enddo

```

Table 7: A very bad choice of C-looping in Fortran. *Do not do this in Fortran.*

```

do I=1,IPART
  do J=1,JPART
    do L=1,LPART
      do N=1,NPART
        ARR(I,J,L,N) = ...
      enddo
    enddo
  enddo
enddo

```

5.10 Stay away from C-code

From the start, the goal has been to keep the Oslo CTM3 free of C-code! Write dummy routines instead; if you need an example, take a look in the directory *OSLO* vs *OSLO/DUMMIES* while you study the *Makefile*.

The only C-code allowed should be in the file *cmn_size.F90* (and of course the DUST code which I have not updated).

5.11 Looping in Fortran

Multidimensional arrays should be traversed in the natural ascending storage order, which is column-major order for Fortran. This means that the leftmost index varies most rapidly with a stride of one. For a loop through the array `ARR(IPAR,JPART)`, the correct traversing is shown in Table 6.

If you want to set the whole array (e.g. initialize it), use

```
ARR(:, :) = 0.
```

not just `ARR = 0.`, which is possible: It makes the code easier to read. If you want to initialize only grid boxes `I=10 to 20` and `J=4 to 10`, you can use `ARR(10:20,4:10) = 0.`. The compiler will chose the most efficient way to handle this.

If you are accustomed to C programming, you should note that C uses row-major order, where the rightmost index varies most rapidly. If you put your 3D or 4D array from C coding into Fortran, it will be very ineffective, striding at every step: If the array is of dimension `(IPAR,JPART,LPART,NPART)`, and you loop through it C-wise, for every step of `N` (from 1 to `NPART`) it must jump (stride) over `IPARxJPARTxLPART` memory locations to get to the next `N` (see Table 7). **You must not do this in Fortran!**

There are of course times when this needs to be violated, for example when rearranging arrays into temporary arrays, with different structures (see e.g. Section 4.3). In cases where the temporary array is smaller, the largest arrays should be traversed in column-major order, to keep the memory jumps as small as possible. Sometimes it may be difficult to decide which way to loop.

5.12 Implicit none

Always use implicit programming, starting each subroutine with `implicit none`. Explicit programming is very difficult to debug if necessary, and should be avoided.

6 Transport

Transport of atmospheric species is done by large scale advection, convection and turbulent mixing. The latter is most important in the boundary layer. The basis for the Oslo CTM3 transport is the Secondary Order Moments scheme introduced by Prather (1986), which was later re-structured and documented in Prather et al. (2008).

6.1 Secondary Order Moments

In addition to transporting mean grid box values, the first and second order moments are also transported. The first order moments carry information about the slope between grid boxes, while the second order moments carry information about the curvature (the slope of the slope).

The 3 first order moments are `SUT`, `SVT` and `SWT`, and the 6 second order moments are called `SUU`, `SVV`, `SWW`, `SUV`, `SUW` and `SVW`. In result, there are 9 moments that need to be transported.

The moment array sizes are `(IPAR,JPART,LPART,NPART)`, and their units are the same as for the mean grid value (i.e. kg/grid box). This may be somewhat counter-intuitive, but is explained in Prather (1986).

The horizontal mass fluxes due to advection is stored in two arrays, one for zonal divergence (`ALFA`) and one for meridional (`BETA`).

```
ALFA(I,J,L) ==> [I,J,L] ==> ALFA(I+1,J,L)
BETA(I,J,L) ==> [I,J,L] ==> BETA(I,J+1,L)
```

Their units are kg/s. See *p-dyn0.f* for more.

It is easy to see that transporting 10 variables per component will require a lot of CPU power, and that the memory requirements also are relatively large. The mass amounts carried by the moments are small compared to the gridbox tracer average (`STT`), and can therefore be stored in single precision (defined by `rMom`). However, in the 1D transport subroutine, everything is carried out in double precision (`r8`). Overall, this makes the code faster, due to reduced code size and hence reduced cache misses. It could be mentioned that conversion from single to double precision takes some extra time, but the gain in a reduced code size is much larger. Comparison

with double precision moments has been done, finding that single precision do introduce some noise, but very small.

6.2 Advection

Advection is carried out through the use of Secondary Order Moments scheme, as described by Prather et al. (2008). The transport papers are available for free at his web page¹.

The global time step is based upon a Lifshitz criterion, which in our case is a divergence criterion (Prather et al., 2008). The transporting routine – `qvect3` – has an internal CFL criteria / time stepping. The latter allows a shorter time step at high latitudes where the grid boxes are smaller compared to low latitudes.

One of the major improvements from Oslo CTM2 is that polar grid boxes are no longer combined in transport (the so-called extended polar zones).

There is, however, one important update from the 2008 description. In Søvde et al. (2012), the treatment of horizontal transport at the polar caps was updated (see Section 6.2.1).

6.2.1 Horizontal advection

The horizontal advection is carried out layer by layer, so that each CPU works on a whole layer. The routines are `DYN2UL` and `DYN2VL`, located in `p-dyn2.f`.

In Prather et al. (2008), the polar cap treatment of horizontal transport was to combine the polar boxes `I` and `I+IPAR/2`, for meridional transport, while maintaining the gradients. This did not work well, and was updated in 2011 to allow for a more accurate treatment, which are described in Søvde et al. (2012).

For meridional transport, the two pie-shaped boxes on opposite sides of the poles are no longer combined, and the V-flux across the pole is zeroed and instead added to the U-flux (transport around the pole point). To avoid short transport time steps due to small masses in the polar-pie grid boxes, the default treatment in Oslo CTM3 is to combine boxes `1:2` and `JPAR-1:JPAR`, for a given `I`, and maintain the moments. An optional, more accurate treatment, is to skip the combining of boxes, but that is more time consuming due to a shorter global time step required in transport. The latter treatment improves cross-polar gradients, and should be considered when studying e.g. frozen-in anti-cyclones or O_3 holes.

To use this optional treatment involves using the files `p-dyn0-v2.f` and `p-dyn2-v2.f` instead of the standard `p-dyn0.f` and `p-dyn2.f`, and is explained in detail in the horizontal transport section of `pmain.f90`.

6.2.2 Vertical advection

The vertical advection is carried out column by column. Large scale advection is computed from the continuity

equation, as the global field `GAMA`. In the IJ-blocks it is put into the field `GAMAB`. Both advection and subsidence due to convection (`GAMACB`) are transported together. I.e. vertical advection must be calculated *after* convection (Section 6.3).

As the advection routine `qvect3` needs the transport pipe to be of *even number length*, care must be taken when using degraded vertical resolution (L37/ or L57) (to get a transport pipe of even length).

There are two possible ways to create even length transport pipes, and for very short arrays (e.g. 19 layers) this may also improve the speed of the vertical advection:

- For each component, stack some columns on top of each other, to be transported as a longer pipe.
- Stack several components from the same column in the longer pipe.

The number of stacked columns or components is given by `IMDIV` in `cmn_size.F90`, and is therefore chosen automatically by `Makefile`.

Due to the model structure, stacking two components from the same column works better than stacking two columns, since the minimum time step needed in the pipe may differ in two columns: Combining different columns means that the column with the shortest time step forces the other columns to take a shorter time step. E.g. convection may cause this, since it can vary much from column to column.

Due to the structure of the B-arrays, this stacking of columns also strides more than for tracer stacking, although that may not be a big problem for computers to handle.

For L60/L40 resolution, the fastest vertical advection is achieved by no stacking at all. For special meteorological conditions using `IMDIV=1` halved the operator splitting time step compared to `IMDIV=4`.

Stacking components has, however, a small disadvantage: If `NPAR` is not divisible with `IMDIV`, the remaining part of the transport pipe will have to be filled with dummy tracers. The cost of this is small. Choosing `IMDIV=2` ensures the least number of dummies.

At some point the cost of creating a long pipe will be larger than the gain of using fewer pipes, reducing the efficiency of this method. For L60 and L40 we use `IMDIV=1`, while for L37 and L57 we use a pipe with 2 components, for both T42 and 1x1 horizontal resolution.

6.3 Convection

Convective transport is calculated as a separate process, and the subsidence due to convection is calculated as a mass flux (`GAMACB`). `GAMACB` is treated together with the large scale vertical advection `GAMA` in the same transport routine (`DYN2W_OC`).

The wet removal of gases due to convective rain is described in Section 7.1.2, whereas the transport is described here.

Convective transport is calculated using mass fluxes of updrafts and downdrafts. The ECMWF IFS convective

¹<http://www.ess.uci.edu/~prather/>

scheme is based on Tiedtke (1989), so we use the same reference for the Oslo CTM3 convection.

Two important processes that occur in convection are entrainment and detrainment. They can be separated into (1) turbulent exchange through cloud edges and (2) organized exchanges. For updrafts the entrainment can be noted

$$E_{up} = E_{up}^{(1)} + E_{up}^{(2)} \quad (14)$$

and detrainment

$$D_{up} = D_{up}^{(1)} + D_{up}^{(2)} \quad (15)$$

If you look at the IFS documentations, you will see that the parameterisations change from cycle to cycle. In general

$$E_{up}^{(1)} = f D_{up}^{(1)} \quad (16)$$

where f may be unity or parameterized. $E_{up}^{(1)}$ is proportional to the incoming mass flux and inverse proportional to the cloud radii:

$$E_{up}^{(1)} = f \frac{0.2}{R_{up}} \frac{M_{up}}{\bar{\rho}} \quad (17)$$

where $\bar{\rho}$ is the air density. In this equation we locate the fractional entrainment (m^{-1}) as:

$$\varepsilon_{up}^{(1)} = \frac{0.2}{R_{up}} \quad (18)$$

See the IFS documentation for more on this and on equations for $E_{up}^{(2)}$ and for detrainment.

Important

While the detrainment rates are given as $[\text{s}^{-1}]$ in the IFS documentation, the meteorological fields available (archived data) are mass flux per height, i.e. accumulated $[\text{kg}/(\text{m}^3\text{s})]$.

Available mass flux fields in the meteorological data are

- Updraft mass flux (CWETE)
- Downdraft mass flux (CWETD)
- Updraft detrainment rate
- Downdraft detrainment rate

The detrainment rates are converted to entrainment mass fluxes CENTU for updrafts and CENTD for downdrafts. See Appendix H.2.1 for some details on this.

For a given grid box, the Oslo CTM3 treatment of convection due to updrafts consists of three parts, considering

- Mass flux in at bottom and out on top.
- Entrainment into updrafts from ambient air.
- Entrainment or detrainment to balance the net updraft mass fluxes and entrainment.

It can be noted that the organized entrainment in the IFS model takes place in the lowest part of the cloud, below the level of strongest vertical ascent (explained in IFS documentation). This information is lost for our use, but the balancing due to net flux will retrieve some of the lost information.

In the convective routine the entrainment CENTU is retrieved as ENT_U and mass flux CWETE as FLUX_E. For a given layer L, with short notation, they are related as

$$F_E(L) + E_U(L) - D_U(L) = F_E(L+1) \quad (19)$$

where F_E is the mass flux from bottom of the given level, E_U is air entrained and D_U is the detrained air at the same level (positive if detrained). In this way we allow detrainment to act as a vent as the air is rising, possibly increasing the mixing with the surrounding air in the process (detrainment will leave polluted mass at lower levels, transporting less to the plume top).

The detrainment $D_U(L)$ is positive when air leaves the convective plume and is lost to the surroundings. From Eq. (19) we have:

$$D_U(L) = -F_E(L+1) + (F_E(L) + E_U(L)) \quad (20)$$

However, it may be that this results in a negative D_U , which means that an additional amount of ambient air needs to be entrained from the surroundings to balance the mass fluxes.

Downdrafts are explained in Appendix H.2.1.

6.4 Boundary layer mixing

The boundary layer mixing scheme is selected by the flag NBLX in *LxxCTM.inp*. In the UCI code only the Prather scheme is available, but in the Oslo CTM3 the Holtslag scheme has been included from qcode 55.

The boundary layer is mixed each chemical time step, before chemistry.

It is important to notice that boundary layer height (BLH) is usually an instantaneous field, which may be problematic during morning hours when photochemistry becomes effective – especially for thin boundary layer heights.

A method for solving this is included, namely interpolating the BLH linearly in time between the current and the next meteorological time step (BLH_CUR and BLH_NEXT, respectively). The routine is called `set_blh_ij`, and is called from `pmain`, in the CCYC-loop. To do this, each IJ-block counts its elapsed seconds of the meteorological time step, in the variable `nmetTimeIntegrated` defined in `pmain`.

Important

This means that when using the time interpolation, BLH should be used with care in other routines.

Except from the boundary layer mixing routine, BLH is put out in several routines (vertical profiles and such), outside the IJ-block. These routines put out values interpolated to each NOPS (if BLH_NEXT is available).

6.4.1 NBLX=1: Prather scheme

The Prather bulk scheme uses e-folding time assuming full mixing in 3 hours. The scheme is set up to be applied to collapsed bottom layers (layer 1 consists of layer 1:3 and layer 2 of 4:5). The bulk scheme should in principle be applicable to the full resolution, but it may be too fast or slow.

It has been tested in the UCI CTM to do well compared with other boundary layer schemes, although much simpler. Some boundary layer parameters are still calculated.

The Oslo CTM3 dry deposition used diffusivities (PBL_KEDDY) for the lowermost model level, which were only calculated in the Holtslag method. A separate calculation of PBL_KEDDY has been included in the Prather scheme.

6.4.2 NBLX=5: Holtslag

The Holtslag et al. (1990) k-profile scheme has been retrieved from the previous version of the UCI model (qcode 55). The boundary layer height needs to be doubled due to catch the whole boundary layer. In L40, a maximum of 9000 m was used, but for L60 this had to be lowered to 8000 m.

```
ZBL = min(BLH(i, J)*2.d0, 8000.d0)
```

6.4.3 Other schemes

No other schemes are available, but qcode 55 also had code for H&R (NBLX=2), Louis (NBLX=3) and M-Y2.5 (NBLX=4).

7 Wet and dry scavenging

Dry deposition is the process where gases are deposited on the ground, i.e. either through gravitational settling or by uptake processes in the soil or in plants. Thus it applies only to the lowermost model level.

Wet deposition, or scavenging, is when gases or aerosols are removed by precipitation.

7.1 Wet scavenging

Wet scavenging is usually divided into three types:

- *Rainout*: Used for aerosols when they act as cloud condensation nuclei (CCN) and fall out as rain.
- *Washout*: Gases/aerosols are deposited on rain drops. This is the usual mechanism for scavenging gases.
- *Sweepout*: When the rain droplets collect molecules or aerosols. Sometimes called *impact washout*.

In Oslo CTM3 we treat washout for both gases and aerosols, since the meteorology (rain) is prescribed: We do not calculate the precipitation from CCN. But the large scale scavenging scheme does also calculate sweepout of species with mass limited washout (i.e. species which easily stick to water, such as HNO_3 and some aerosols), called impact washout in the code.

It should be noted that the washout process is treated differently for large scale and convective precipitation.

The wet scavenging parameters are found in the file *scavenging_wet.dat*, as listed in Tables 32–34. It differs from the original UCI file, which is also available in *scavng55.dat* for the interested reader. In general, the scavenging follows Henry's law, so coefficients for this are

listed. How to specify more sophisticated effective expressions is explained in Section 7.1.4. The settings apply in general to the large scale wet scavenging, but there are a few options that only apply for convective scavenging.

The wet scavenging list contains parameters for convective scavenging and large scale scavenging – where some are specific for either convective or large scale, but most apply for both. Here follows a list of the parameters, which are also described at the end of the scavenging list.

- **SOLU**: Fraction of grid box available for wet scavenging. Applies for both convective and large scale scavenging. For convective scavenging, this must be accompanied by setting the flag **CHN**
- **CHN**: Defines treatment of convective scavenging, with the possibility to switch off liquid or ice large scale scavenging. Options are listed at the bottom of the scavenging file, and the most used flags are 0, 1 or 3. Large scale scavenging is treated unless stated otherwise:

- 0 No convective scavenging.
- 1 Fraction dissolved is calculated from Henry coefficients, either using Henry's law or mass-limited. This fraction is multiplied with **QFRAC** to get the fraction removed by scavenging (Section 7.1.2–7.1.3).
- 2 Not in use.
- 3 Assumes fully dissolved tracer, so that **QFRAC** gives the fraction removed.
- 4 Removes fraction given by **SOLU** and *not* **QFRAC**. In other words: Everything is removed for **SOLU**=1. Should be used with care!
- 5 Same as (3), but large scale scavenging is turned off.
- 6 Same as (3), but large scale scavenging on liquid is turned off. Large scale ice scavenging is included (if defined by **ISCVFR**).
- 7 Convective removal only if minimum temperature in convective plume is lower than 258 K. Large scale ice scavenging is included, but not liquid scavenging.
- 8 Convective removal only if minimum temperature in convective plume is lower than 258 K and maximum temperature in plume is lower than 273 K. Large scale ice scavenging is included, but not liquid scavenging.

- **TCHENA**: First part of Henry expression, i.e. Henry coefficient at 298 K.
- **TCHENB**: Exponential part of Henry expression, i.e. the temperature coefficient.
- **TCKAQA**: Flag for denoting that Henry expression should be modified by hard-coded settings. See 7.1.4 for more.
- **TCKAQB**: Zero is removal according to Henry expression, non-zero is mass (or kinetically) limited removal, which is used for highly soluble species.
- **ISCVFR**: Fraction of gridbox available for large-scale ice scavenging.
- **IT**: Ice treatment when **ISCVFR**>0.

- 0 No scavenging below 258 K.
- 1 For temperatures below 258 K use Kärcher and Voigt (2006).
- 2 Use same treatment as for 258 K–273 K, i.e. with retention coefficient.

- 3 No removal for $T < 258$ K, but set retention coefficient to 1 instead of 0.5.
- 4 Standard treatment (Henry's law or kinetically limited) below 258 K (as in option 2), but set retention coefficient to 1 instead of 0.5.

7.1.1 Large scale scavenging

The large scale scavenging master routine located in `WASHOUT0`. While the model in principle can use a simplified scheme (`WASHOUT1`), it has been disabled for Oslo CTM3; we only use the more sophisticated version by Neu and Prather (2012) (`WASHOUT2`), which scavenge separately by liquid and ice precipitation. It is still possible to choose the simple scheme by changing the parameter `NSCX` in the input file `LxxCTM.inp`, but the data needed is not read into the model. If you need that data, you can find it in `scavng55.dat`.

The `WASHOUT2` is a simple cloud model, dividing each grid box layer in four parts:

- Cloud core, with rain coming in from above. Depending on how much rains out, rain may evaporate or be formed.
- Cloudy, with no rain coming in, but rain may form.
- Clear sky with rain from above.
- Clear sky with no rain.

Fractional areas are calculated and may change e.g. due to evaporation. A constant evaporation rate is used. More details are explained by Neu and Prather (2012).

For some species, such as HNO_3 and some aerosols, uptake on ice may be important. Uptake on ice is controlled by a non-zero ice scavenging fraction `ISCVFR` in the scavenging list, denoting how much of the grid box is available for ice scavenging. For $258 \text{ K} < T < 273 \text{ K}$, the uptake is generally calculated using Henry's law and the table-specified Henry's law coefficients, modified by a retention coefficient. This is because Henry expressions are not given for temperatures below 0°C , and currently the retention coefficient is set to 0.5 (Neu and Prather, 2012). Mass limited ice removal of species is calculated assuming a Henry coefficient of typically 10^8 , which will yield the species completely dissolved, even if the retention coefficient is 0.5.

Note that the retention coefficient can possibly be overwritten by the IT flags. In the future, it could be that the retention coefficient could become part of the scavenging table.

Uptake of HNO_3 on ice can also occur below 258 K, and follows Kärcher and Voigt (2006) when IT is set to 1. Other options are also available.

7.1.2 Convective scavenging

Convective scavenging is adopted from the Oslo CTM2, and does not separate between ice and liquid water; all is treated as rain. It differs from the UCI method, which is rather crude. The routines are called from `CONVW_0C` and are located in `cnv_oslo.f90`.

If you need to do changes in that file, be certain that you understand the units used; rain, liquid water and mass

fluxes are kg/s. Note that these values are accumulated in the meteorological data files, and then converted. Entrainment into updrafts is originally not flux, and is described in Section 6.3.

Convection forms an elevator (or plume) transporting mass upwards. To calculate the convective scavenging we need to know how much of a tracer that is solved in the liquid water of the elevator (`elev_mass_lw`), which is described at the end of this section. The `elev_mass_lw` also covers the rain in the elevator.

The fraction of rain to liquid water in the elevator is called `QFRAC`. Given an amount of tracer solved in the elevator liquid water, the fraction `QFRAC` is subject for removal.

Calculation is done using the mass fluxes from the meteorological data. At the lowest level of entrainment, we entrain air and humidity from the surroundings, to form the base of the elevator. It is then lifted according to the mass fluxes, and assuming adiabatic lifting, the elevator temperature cools and eventually water will condense. The condensed water goes into `elev_mass_lw`. Entrainment or detrainment is then calculated, before we remove the net rain out of the box. We do not consider net rain into the box to increase `elev_mass_lw`; with our simplified elevator, this unfortunately not possible.

Eventually we reach the elevator top (determined by the mass fluxes) and we have the following data for each level of the elevator: Amount of liquid water, volume of elevator and volume fraction of liquid water (droplets) in the elevator, which is called `LW_VOLCONC` (e.g. volume concentration). `LW_VOLCONC` is used in calculating the amount of tracer solved in the elevator. Some species are dissolved completely (e.g. HNO_3) and others are dissolved according to Henry's law (Section 7.1.3).

In the scavenging list, the parameters `SOLU` and `CHN` defines whether or not each tracer is washed out by convection. These data are stored in the model arrays `TCWETL(NPAR)` and `TCCNVHENRY(NPAR)`, respectively. `CHN` controls how to calculate the fraction of tracer removed. Options are listed at the bottom of the scavenging file, and also in the previous Section.

The use of Henry's law to find the fraction of tracer dissolved in the elevator is described in the next Section.

7.1.3 Theory on Henry's law

Looking at the convective scavenging code, you find a fraction of dissolved tracer on the form

$$f_{dissolved} = \frac{H_H LW_{volconc}}{H_H LW_{volconc} + 1} \quad (21)$$

A similar expression can be found in the large scale scavenging routine (subroutine `HENRYS`, although it is different below 273 K). I will explain the background of this equation here.

First of all, there are several data on Henry coefficients; usually they are given at 298 K, together with a temperature coefficient. Another possibility, as in Sander et al. (2011), coefficients are given for the expression:

$$\ln H(T) = A + \frac{B}{T} + C \ln T \quad (22)$$

Coefficient C is rarely used, and while B is used by the Oslo CTM3, I stress that this A -coefficient differs from the model definition: Oslo CTM3 applies the well used van't Hoff's temperature extrapolation from 298 K. This extrapolation assumes that Henry's law varies as

$$\frac{d \ln H}{dT} = \frac{\Delta H_{sol}}{RT^2} \quad (23)$$

where ΔH_{sol} is the solution enthalpy. ΔH_{sol} is assumed constant (a fairly good approximation), so that the expression can be re-arranged and integrated between temperatures T_1 and T_2 :

$$H(T_2) = H(T_1) \exp \left[\frac{\Delta H_{sol}}{R} \left(\frac{1}{T_1} - \frac{1}{T_2} \right) \right] \quad (24)$$

The temperature dependence

$$\frac{\Delta H_{sol}}{R} = - \frac{d \ln H}{d(\frac{1}{T})} \quad (25)$$

is the B coefficient given e.g. by Sander et al. (2011) and also used in the Oslo CTM3. Hence, using $T_2 = 298$ K, the model finds the Henry expression at any temperature:

$$H(T) = H(298 \text{ K}) \exp \left[B \left(\frac{1}{T} - \frac{1}{298 \text{ K}} \right) \right] \quad (26)$$

This means that the A -coefficient used in the model (in scavenging table), is in fact $H(298 \text{ K})$.

The following explanation applies to the convective scavenging, where $LW_{volconc}$ is calculated. In the routine for large scale scavenging, $LW_{volconc}$ is not explicitly calculated, which is why Eq. (21) differs slightly in that routine. However, the basics behind it is the same.

Important notice

When Eq. (21) is used and $LW_{volconc}$ is calculated, as in the convective routine, $H(T)$ has to be modified to get the correct units, i.e. we have to multiply it by RT , where $R = 0.08206 \text{ atm L mol}^{-1} \text{ K}^{-1}$.

Deriving Eq. (21)

Henry's law coefficient for any gas is defined as

$$P_{gas} = k_H X \quad (27)$$

where P_{gas} is the partial pressure of the gas above the solution, and X is the molar fraction of the dissolved gas in the solution;

$$X = \frac{n_{aq}}{n_{aq} + n_{solvent}} \quad (28)$$

where n_{aq} is the number of moles solved, and $n_{solvent}$ is the number of moles of the solvent (i.e. water in our case).

Assuming ideal solution, we can change to concentration by dividing by volume of the solution, and get:

$$X = \frac{C_{aq}}{C_{aq} + C_{solvent}} \quad (29)$$

As long as Henry's law applies, i.e. the species is *not* highly soluble, we always have $C_{aq} \ll C_{solvent}$, and can approximate to:

$$X = \frac{C_{aq}}{C_{solvent}} \quad (30)$$

Since the concentration of the solvent (water) is approximately constant, we arrive at the other common form of Henry's law:

$$P_{gas} = k C_{aq} \quad (31)$$

Units for k : $[\text{atm L(solvent)}/\text{mol}]$, and for P_{gas} : $[\text{atm}]$.

If k is high, it means the component prefers thermodynamically to be in gas phase.

We are interested in calculating C_{aq} from P_{gas} , so we introduce

$$H_{STAR} = 1/k \quad (32)$$

with units $[\text{mol}/(\text{atm L(solvent)})]$, so that

$$C_{aq} = H_{STAR} P_{gas} \quad (33)$$

If we want to apply the calculations to molar concentration (mol/L), we have to change some units:

$$P_{gas} = C_g RT \quad (34)$$

given correct units of R , i.e. $[\text{atm L}/(\text{mol K})]$:

- $J = \text{kg m}^2/\text{s}^2 = \text{Pa m}^3$
- $R = 8.31451 \text{ J}/(\text{mol K}) / 101325 \text{ Pa/atm} \times 1000 \text{ L/m}^3 = 0.0820578 \text{ atm L}/(\text{mol K})$

Henry's law therefore implies that the concentration in the solution is proportional to the atmospheric concentration:

$$C_{aq} = H_{STAR} R T C_g = H_H C_g \quad (35)$$

where H_H has the units $[\text{mol/L(solvent)} / (\text{mol/L(air)})]$.

We want the mass fraction of the dissolved gas, which equals the molar fraction $f_{dissolved}$.

$$f_{dissolved} = \frac{n_{aq}}{n_{aq} + n_g} \quad (36)$$

The volumes have units $[\text{m}^3]$, while the number concentration of tracer in air, C_g , has units $[\text{mol/L(air)}]$. Hence, we get the moles of tracer in gas phase:

$$n_g = C_g V_{elevator_air} \frac{10^3 \text{ L(air)}}{\text{m}^3(\text{air})} \quad (37)$$

C_{aq} has units $[\text{mol/L(solvent)}]$, and the number of moles in the solution is

$$n_{aq} = C_{aq} V_{elevator_solvent} \cdot 10^3 \text{ L(solvent)}/\text{m}^3(\text{solvent}) \quad (38)$$

As already explained, the solvent is liquid water. The volume of the solvent is given by the liquid water content, and is calculated in elevator fractions as volume concentration, i.e. volume of liquid water in elevator to total elevator volume. As can be found in the source code comments, the volume of liquid water is

$$V_{elevator_solvent} = \frac{\text{mass of liquid water}}{\rho} \quad (39)$$

where ρ is the density of water (which is 10^3 kg/m^3). The liquid water volume concentration is then

$$LW_{volconc} = \frac{V_{elevator_solvent}}{V_{elevator_air}} \quad (40)$$

Using Equation (38) and (40), the moles of gas dissolved in water is

$$n_{aq} = C_{aq} LW_{volconc} V_{elevator_air} \quad (41)$$

$$\cdot 10^3 \text{ L(solvent)}/\text{m}^3(\text{solvent}) \quad (42)$$

The mass fraction dissolved in the droplets (mass fraction equals mole fraction in this case), which is subject to washout, is therefore

$$\begin{aligned} f_{dissolved} &= \frac{n_{aq}}{n_{aq} + n_g} \\ &= \frac{C_{aq}LW_{volconc}}{C_{aq}LW_{volconc} + C_g} \end{aligned} \quad (43)$$

and by Equation (35) we get

$$f_{dissolved} = \frac{H_H LW_{volconc}}{H_H LW_{volconc} + 1} \quad (44)$$

In the Oslo CTM3 code this fraction is called `DISSOLVEDFRAC`.

When the retention coefficient is used in large scale scavenging, it is multiplied by H_H in Equation (44).

7.1.4 Hard-coded Henry coefficients

Some tracers have empirical Henry constants, which need to be hard-coded. This is specified by a non-zero `TCKAQA` in the scavenging list *scavenging_wet.dat*.

The hard coding is done in the routine `getHstar` in *scavenging_largescale_uci.f90*, called by either the large scale scavenging routine or the convective scavenging routine.

7.2 Dry deposition

Deposition velocities are stored in `VDEP` of size `(NPAR,IPAR,JPAR)`, thus allowing for possible deposition of any transported tracer.

`VDEP` is given in units [m/s], and is set in subroutine `setdrydep` in the file *drydeposition_oslo.f90*, which is called from `pmain`.

Important

When these deposition velocities are to be used in `QSSA`, they have to be divided by the height of the lowermost layer, to get the unit [s⁻¹]. This is carried out e.g. before chemistry (`MASTER_OSLO`) and in subroutine `bcoc_master`.

Important 2

The dry deposition parameterisation is in the process of being updated, so we still stick to the Oslo CTM2 parameterisation. It is explained very briefly in Section 7.2.1, while the new scheme is described in Section 7.2.2–7.2.3.

7.2.1 Historical note

In the Oslo CTM3 (Søvde et al., 2012) and its predecessor Oslo CTM2 dry deposition has been parameterised based on Wesely (1989), not by calculating the deposition velocities from equations, but rather by using seasonal day and night averaged deposition velocities for different land use types. However, some velocities seem to rather come from Hough (1991).

Using 5 land-use types (water, forest, grass, tundra/desert and ice/snow) in each gridbox, a mean velocity was then defined. Day and night was defined by

using the solar zenith angle (subroutine `SOLARZ`), giving day if less than 90°. Winter was defined as temperatures below 273.15 K for grid boxes containing land masses. Ocean gridboxes containing sea ice use ice/snow values, but a distinction on season was not necessary because the summer and winter values are equal. However, snow cover was taken into account, reducing uptake when snow thickness was about 1 m (10 cm water equivalents) in forest and 10 cm (1 cm water equivalents) on grass/tundra.

7.2.2 The new dry deposition scheme

The dry deposition parameterisation is in the process of being updated to follow the method of the EMEP model (Simpson et al., 2012). It is a more physical approach and is described in detail in Section 7.2.3.

The EMEP method is used for the gaseous species O_3 , H_2O_2 , NO_2 , PAN , SO_2 , NH_3 , $HCHO$, CH_3CHO . CO has a very small uptake and is not included in the EMEP treatment, so we keep the old Oslo CTM2 parameterisation.

Some of the aerosol deposition rates follow the EMEP aerosol parameterisation, namely BC/OC aerosols, sulphur aerosols (SO_4 and MSA), and secondary organic aerosols (SOA). Other aerosol modules have their own parameterisations which are described in their own sections of this manual.

This paragraph will be rewritten – do not read it
Compared to the old scheme, the new parameterisation improves the ability to reproduce measured surface O_3 . Generally, the largest impacts can be found for O_3 , HNO_3 , SO_2 and NH_3 , but also for SO_4 due to changes in SO_2 . Tropospheric burden of O_3 and HNO_3 increases by 5–8 % and 5–10 %, respectively. A ~20 % decrease is found for tropospheric SO_2 and SO_4 , while NH_3 tropospheric burden decreases by 20–30 %. The other species do not change much (0–3 %). Interestingly, NO_2 decreases slightly during winter but increases more during summer, showing that secondary effects coming from chemistry are also important.

The old UCI read-in is disabled, but a short note about it is given in Section 7.2.7.

7.2.3 Technical description: gaseous species

Typically, deposition uptake follows an electric circuit analogy, where the deposition velocity v_d^i for species i is

$$v_d^i = \frac{1}{R_a + R_b^i + R_c^i} \quad (45)$$

where R_a is the aerodynamical resistance between the surface and the top of the vegetation canopy (i.e. the altitude z_0 , called roughness length), R_b^i is the quasi-laminar layer resistance to the gas and R_c^i is the canopy resistance (often called surface resistance and sometimes denoted r_s^i).

R_a is the same for all gases, depending only on the surface/air properties. R_b^i and R_c^i are different for all gases, and the latter also vary from vegetation type to vegetation type.

The inverse of a resistance is called conductance, which is denoted G :

$$G = \frac{1}{R} \quad (46)$$

Conductance is in essence the same as velocity. This is important to keep in mind when calculating an average deposition value in a gridbox.

If Eq. (45) is the gridbox average, then the R s are grid box averages. This must be kept in mind when calculating grid box averages of R_c^i , which depend on land-use types; then we need to calculate resistances for all vegetation types and do a proper weighting to get the gridbox average.

To do this weighting we assume that a molecule can only choose one land type; it will not take the least resistance of several land-use types.

As an example, assume we have 2 land-use types with gridbox fractions being 20 % and 80 %, respectively, with resistances $R_1 = 1000$ s/m and $R_2 = 100$ s/m. A molecule is located above one of these surfaces and cannot choose where to go. This assumption means that several land-use types, e.g. forest and grass, cannot occupy the same area when the area is infinitesimally small (approaches zero).

Then the gridbox average R is found by

$$\frac{1}{R} = 0.2 \cdot \frac{1}{R_1} + 0.8 \cdot \frac{1}{R_2} \quad (47)$$

or from conductances

$$G = 0.2 \cdot G_1 + 0.8 \cdot G_2 \quad (48)$$

This is perhaps more easily explained using velocities: If 20 % of the gridbox has deposition velocity of 10^{-3} m/s and the 80 % part has 10^{-2} m/s, the land-use fraction weighted mean is 0.0082 m/s. If you erroneously calculated the mean $R = 0.2R_1 + 0.8R_2$ you would get the velocity 0.00357 m/s.

Hence, it is the velocities (or conductances) which have to be weighted according to land-use fractions, to get a gridbox mean velocity.

The new dry deposition scheme calculates R_a , R_b^i and R_c^i following Simpson et al. (2012), which will be referred to as EMEP2012. Main gases included are O_3 , SO_2 , NH_3 , NO_2 , H_2O_2 and HNO_3 , but in addition I have included NO , $HCHO$ and CH_3CHO which to some extent are also subject to dry deposition.

As already noted, dry deposition of CO is still treated with the old scheme. This is because it is not available through EMEP2012. In general, CO dry deposition is so small that models tend to exclude it. It is set to 0.03 cm/s over vegetated areas Conrad and Seiler (1985), and it is reduced when there is snow.

Aerosols are not part of the new update and follows the old deposition treatment, using fixed deposition velocities or calculated separately as in the sea salt or mineral dust modules.

Important

To use this treatment, both the nitrate and sulphur modules should be included. They are needed for calculation

of SO_2 deposition which is again needed to calculate dry deposition velocities for other gases. Note that Søyde et al. (2012) concluded that these modules should be included anyway; doing so does not increase computing time by much. Still, if sulphur and nitrate are not included, a monthly model climatology of the parameters a_{sn} and a_{sn}^{24h} is needed.

However, this climatology has not yet been produced, so if you try to run the model without sulphur and nitrate modules, the program will stop.

Aerodynamical resistance R_a

The aerodynamical resistance (R_a) in EMEP2012 is not well defined in Simpson et al. (2012). They first assess friction velocity u_* by using stability functions (Eq. (52) in EMEP2012):

$$u_* = \frac{V_H(z) k}{\ln\left(\frac{z-d}{z_0}\right) - \Psi_m\left(\frac{z-d}{z_0}\right) - \Psi_m\left(\frac{z_0}{L}\right)} \quad (49)$$

Here, $V_H(z)$ is the wind speed at their reference height z and Ψ_m represents the integrated stability equations for momentum, d is a constant (typically 0.7 m), and L is the Obukhov length. However, they do not list the equation for R_a .

A somewhat similar expression is found for R_a in the earlier EMEP version (EMEP2003, Simpson et al., 2003), namely

$$R_a = \frac{1}{k u_*} \left[\ln\left(\frac{z-d}{z_0}\right) - \Psi_h\left(\frac{z-d}{z_0}\right) - \Psi_h\left(\frac{z_0}{L}\right) \right] \quad (50)$$

However, for certain values of z , z_0 and L , Eq. (50) can produce a negative R_a , which is wrong. This also applies to the u_* calculation of EMEP2012.

Therefore we use a different approach in Oslo CTM3, namely the method of Monteith (1973). Sensible heat flux (SHF) between surface and air is given by

$$SHF = \rho c_p \frac{T_0 - T_z}{R_{a,H}} \quad (51)$$

where ρ is air density, c_p the specific heat at constant pressure, T_0 is the surface temperature, T_z is the temperature at reference height z , and the aerodynamic resistance $R_{a,H}$ is the diffusion resistance to sensible heat transfer between surface and the reference height z . In Oslo CTM3 it is assumed that $R_a = R_{a,H}$.

Sensible heat flux can also be written

$$SHF = -\rho c_p K_H \frac{\partial T}{\partial z} \quad (52)$$

and momentum flux using the wind u profile

$$MF = -\rho u_*^2 = \rho K_M \frac{\partial u}{\partial z} \quad (53)$$

where K_H and K_M are the respective eddy diffusivities. When $K_M = K_H$, Eq. (52) and (53) gives

$$SHF = -\rho c_p \frac{\partial T}{\partial u} u_*^2 \quad (54)$$

which in finite differences between surface and reference height z can be written

$$SHF = \rho c_p (T_0 - T_z) \frac{u_*^2}{u_z} \quad (55)$$

where T_z and u_z are temperature and wind speed at height z . From Eq. (51) we get the Monteith (1973) equation for $R_{a,H}$:

$$R_{a,H} = \frac{u_z}{u_*^2} \quad (56)$$

This is what we use for R_a in Oslo CTM3, and as reference height we use the midpoint of the surface model level. This level is about 16 m thick, so the reference height is about 8 m. This is possible because both u_z and u_* are available from the meteorological data.

Quasi-laminar layer resistance R_b

R_b^i is species specific, and is defined differently over land and ocean. When a gridbox contain both land and ocean, a weighted mean R_b^i is calculated using the respective land and ocean conductances.

Over land we use

$$R_b^i = \frac{2}{k u_*} \left(\frac{Sc_i}{Pr} \right)^{2/3} \quad (57)$$

where Pr is the Prandtl number (0.72) and Sc_i is the Schmidt number for gas i , defined as:

$$Sc_i = \frac{\nu}{D_i} \quad (58)$$

Here ν is the kinetic viscosity of air and D_i is the molecular diffusivity for gas i . If you look at the code, you will see that the $Sc_{H_2O} = 0.6$ as well as $D_{H_2O} = 0.21 \cdot 10^{-4}$ are defined, and that Sc_i is found from

$$Sc_i = Sc_{H_2O} \frac{D_{H_2O}}{D_i} \quad (59)$$

where D_{H_2O}/D_i is listed in Table 8.

Over sea we use

$$R_b^i = \frac{1}{k u_*} \ln \left(\frac{z_0}{D_i} k u_* \right) \quad (60)$$

with minimum limit of 10 s/m and maximum of 1000 s/m.

z_0 is available from monthly mean ISLSCP2/FASIR but have zero value over ocean. Hence, a different approach is taken to find z_0 over water; assuming different approaches over calm and rough ocean, separated by wind speed of 3 m/s. Calm sea follows e.g. Hinze (1975) or Garratt (1992), but with a slightly higher coefficient:

$$z_{0,w,calm} = \min \left(2 \cdot 10^{-3}, 0.135 \frac{\nu}{u_*} \right) \quad (61)$$

where ν is kinematic viscosity for air, calculated from surface pressure (P_{sfc}), temperature (2-meter temperature T_{2M}) and gas constant for air (R_{air}):

$$\nu = \frac{6.2 \cdot 10^{-8} T_{2M}}{\frac{P_{sfc}}{T_{2M} R_{air}}} \quad (62)$$

Here the numerator is absolute viscosity and the denominator is air density.

Rough sea follows the method of Wu (1980), which is the Charnock (1955) method with slightly higher coefficient.

$$z_{0,w,rough} = \min \left(2 \cdot 10^{-3}, 0.018 \frac{u_*^2}{g} \right) \quad (63)$$

In addition, there is a maximum roughness length limit of 2 mm imposed on both cases. However, the calculated

Table 8: Values of D_{H_2O}/D_i and f_0^i and H_*^i .

| Species i | D_{H_2O}/D_i | f_0^i | H_*^i [M/atm] |
|-------------------------------|----------------|---------|-------------------|
| O ₃ | 1.6 | 1.0 | 10^{-2} |
| SO ₂ | 1.9 | 0.0 | 10^5 |
| NO ₂ | 1.6 | 0.1 | 10^{-2} |
| H ₂ O ₂ | 1.4 | 1.0 | 10^5 |
| HCHO | 1.3 | 0.0 | $6 \cdot 10^3$ |
| NO | 1.3 | 0.0 | $2 \cdot 10^{-3}$ |
| CH ₃ CHO | 1.6 | 15.0 | 0.0 |

$z_{0,w}$ is usually so small that the limits on Eq. (60) kicks in, so in practice $z_{0,w}$ could very often have been zero in this parameterisation.

Surface resistance R_c

Surface resistance (R_c^i) consists of both stomatal and non-stomatal resistances. To find the gridbox average we use conductances, as explained earlier:

$$G_c^i = LAI \cdot G_{sto} + G_{ns}^i \quad (64)$$

where LAI is the leaf area index (zero for non-vegetated surfaces), G_{sto} is the stomatal conductance and G_{ns}^i is the non-stomatal conductance.

We use monthly mean LAI from ISLSCP2/FASIR and G_{sto} from the LPJ group (provided through HYMN project).

Stomatal conductance

Note that EMEP2012 calculate G_{sto} from a maximum stomatal conductance g_{sto} multiplied by functions to take temperature, light, etc. into account. This is not necessary when we have monthly mean values.

However, we do a scaling based on the photosynthetically active radiation (PAR) available through the meteorological data, multiplying G_{sto} at each time step (and grid box) with PAR and dividing by the monthly mean:

$$G_{sto}(t) = G_{sto} \frac{PAR(t)}{PAR_{mean}} \quad (65)$$

I.e. both PAR and PAR_{mean} are given in each gridbox. This ensures a daily variation and also that the monthly average G_{sto} is maintained.

It could be that there should be a lower limit on PAR in Eqn (65), e.g. 200 Wm^{-2} , because stomata does not open immediately when the sun rises. If so, the PAR_{mean} should be re-generated with this assumption.

Non-stomatal conductance

In the new scheme, non-stomatal conductance is calculated specifically for O₃, SO₂, HNO₃ and NH₃. For other species, an interpolation between O₃ and SO₂ values are carried out.

– O₃ –

The non-stomatal conductance for O₃ consists of two terms, one depending on vegetation type and one depending on the soil/surface. For land-type N of N_{max} types, we can write:

$$G_{ns}^{O_3}(N) = \frac{SAI(N)}{r_{ext}} + \frac{1}{R_{inc}(N) + R_{gs}^{O_3}(N)} \quad (66)$$

$SAI(N)$ is the surface area index for vegetation type N , which is LAI plus some value representing cuticles and

other surfaces, having external leaf resistance of $r_{ext} = 2000 F_T \text{ s/m}$, where F_T is a temperature correction factor for temperatures below -1°C . Note that F_T has an upper limit of 2, hence has a range of 1–2:

$$F_T = \exp(-0.2(1 + T_s)) \quad ; \quad 1 \leq F_T \leq 2 \quad (67)$$

We assume that T_s in this equation is the surface temperature, i.e. 2-meter temperature T_{2M} . Temperature unit is $^\circ\text{C}$.

In general we have that $SAI = LAI$ for all land types, but there are three exceptions. The first two exceptions are forest and wetlands, for which we set $SAI = LAI + 1$. The last exception is for cropland; during the first part of the growth season $SAI = LAI \cdot 5/3.5$ while for the second part $SAI = LAI + 1.5$. In winter, cropland act as a non-vegetated surface with $SAI = 0$.

The two parts of growth seasons are simply defined:
NH: day 90–140 and 141–270.
SH: day 272–322 and 323–452 (i.e. day 87).

In this way, vegetation affects the conductance also by being there, not only by uptake through the stomata.

R_{inc} is the in-canopy resistance, defined for each vegetated land-type N as

$$R_{inc}(N) = b SAI(N) \frac{h(N)}{u_*} \quad (68)$$

where $h(N)$ is the canopy height and $b = 14 \text{ s}^{-1}$ is an empirical constant. The in-canopy resistance is not affected by temperature or snow in EMEP2012, and is of course zero for non-vegetated surfaces.

The term $R_{gs}^{O_3}(N)$ is found from tabulated values of all land-types ($\hat{R}_{gs}^{O_3}$), corrected by F_T and snow cover $f_{snow}(N)$:

$$\frac{1}{R_{ns}^{O_3}(N)} = \frac{1 - f_{snow}(N)}{\hat{R}_{ns}^{O_3}(N)} + \frac{f_{snow}(N)}{R_{snow}^{O_3}} \quad (69)$$

Note that EMEP2012 uses $2f_{snow}$ with a range of $[0,1]$. This is explained weirdly in Zhang et al. (2003), but we stick to using f_{snow} with range $[0,1]$.

Table 9 lists all land-use types and according values of $h(N)$, $SAI(N)$, $\hat{R}_{ns}^{O_3}(N)$ and $\hat{R}_{ns}^{SO_2}(N)$. Forest vegetation height is assumed to be 20 m up to 60 degrees latitude, and 6 m poleward of 75 degrees. From latitudes 60–75 a linear interpolation is carried out.

Snow cover

Snow cover does complicate the treatment slightly, because it depends on the land-type category: While e.g. 10 cm of snow may be enough to cover grass, it is not enough to cover forest. So we calculate a snow cover fraction using the snow depth S_D available through the meteorological data (note that this is given in meter equivalent water, so we multiply by 10 to get snow depth in meter):

$$f_{snow}(N) = \frac{S_D}{S_{D,max}} = \frac{10 S_D}{0.1 h(N)} \quad (70)$$

This is carried out for each land-type, under the simple assumption that $S_{D,max} = 0.1 h(N)$, where $h(N)$ is the canopy height for the given land-type N . For O_3 we assuming $R_{snow}^{O_3} = 2000 \text{ s/m}$ as in EMEP2012, constant for all temperatures.

Table 9: Land-use properties in the new dry deposition treatment.

| | Vegetation | $\hat{R}_c^{O_3}$ | $\hat{R}_c^{SO_2}$ | SAI | h [m] |
|--|------------|-------------------|--------------------|-------|-------|
| 1 | Forest | 200 | – | LAI+1 | 20* |
| 2 | Crops | 200 | – | ◇ | 0.4 |
| 3 | Moorland | 400 | – | LAI | 0.7 |
| 4 | Grassland | 1000 | – | LAI | 0.4 |
| 5 | Wetland | 400 | 50 | LAI+1 | 0.5 |
| 6 | Tundra | 400 | 500 | LAI | 0 |
| 7 | Desert | 2000 | 1000 | 0 | 0 |
| 8 | Water | 2000 | 1 | 0 | 0 |
| 9 | Urban | 400 | 400 | 0 | 0 |
| 10 | Snow/ice | 2000 | 1000 | 0 | 0 |
| –: Calculated, see text. | | | | | |
| *: 20 m up to 60 N/S, 6 m from 75 N/S. | | | | | |
| Interpolated 60–75 N/S. | | | | | |
| ◇: Season dependent, see text. | | | | | |

From the equations above, we see that this means that both the SAI -term and R_{inc} are unaffected by temperature and snow.

Adding it up

For each land-use type N we now calculate $G_{ns}^{O_3}(N)$ according to Eq. (66) using the land-type specific SAI , R_{inc} and $\hat{R}_{gs}^{O_3}$ corrected by F_T and f_{snow} . Then we make a gridbox average using the according land-type fractions (f_L):

$$G_{ns,tot}^{O_3} = \sum_{N=0}^{N_{max}} G_{ns}^{O_3}(N) \cdot f_L(N) \quad (71)$$

Finally, we have the gridbox average $R_c^{O_3}$:

$$R_c^{O_3} = \frac{1}{LAI \cdot G_{sto}^{O_3} + G_{ns,tot}^{O_3}} \quad (72)$$

– NH_3 –

$R_c^{NH_3}$ is treated separately using the molar ratio of SO_2/NH_3 :

$$a_{sn} = \frac{[\text{SO}_2]}{[\text{NH}_3]} \quad (73)$$

An upper limit of 10 is assumed, and this limit is also used for $[\text{NH}_3]=0$. Using the 2 m temperature (T_{2M}) we have that for $T_{2M} > 0^\circ\text{C}$:

$$R_c^{NH_3} = \beta F_1(T_{2M}, RH) F_2(a_{sn}) \quad (74)$$

where $\beta = 1/22$ is a normalising factor, and

$$F_1 = 10 \log_{10}(T_{2M} + 2) \exp\left(\frac{100 - RH}{7}\right) \quad (75)$$

where RH is relative humidity in percent, and

$$F_2 = 10^{-1.1099 a_{sn} + 1.6769} \quad (76)$$

See Simpson et al. (2012) for references.

If you run the Oslo CTM3 without the nitrate and sulphur modules, a_{sn} should be read from a monthly model climatology.

– SO₂ –

The EMEP2012 treatment is based on an empirical formula for vegetated surfaces, using the 24 hour mean molar ratio of SO₂/NH₃ (a_{sn}^{24h}):

$$R_{ns}^{SO_2} = 11.84 \exp(1.1 a_{sn}^{24h}) f_{RH}^{-1.67} \quad (77)$$

Here a_{sn}^{24h} is limited to 3, and f_{RH} is fractional humidity (0–1). Minimum and maximum limits of 10 s/m and 1000 s/m, respectively, are imposed, and if $f_{RH} = 0$ we assume maximum value.

Additionally, there is a temperature dependent limit for SO₂, using the 2 m temperature (T_{2M}):

$$R_{ns}^{SO_2} = 500 \text{ s/m for } T_{2M} \leq -5^\circ\text{C} \text{ and } R_{ns}^{SO_2} = 100 \text{ s/m for } -5^\circ\text{C} < T_{2M} \leq 0^\circ\text{C}.$$

For non-vegetated land surfaces, tabulated values $\hat{R}_{ns}^{SO_2}(N)$ are used (Table 9, modified with F_T similarly as explained for O₃):

$$\frac{1}{R_{ns}^{SO_2}(N)} = \frac{1 - f_{snow}(N)}{\hat{R}_{ns}^{SO_2}(N)} + \frac{f_{snow}(N)}{R_{snow}^{SO_2}} \quad (78)$$

Here we have

$$\begin{aligned} R_{snow}^{SO_2} &= 70 & T_{2M} \leq +1^\circ\text{C} \\ &= 70 \cdot (2 - T_{2M}) & -1^\circ\text{C} \leq T_{2M} < +1^\circ\text{C} \\ &= 700 & T_{2M} \leq -1^\circ\text{C} \end{aligned} \quad (79)$$

The total conductance is then

$$G_{ns,tot}^{SO_2} = \sum_{N=0}^{N_{max}} \frac{1}{R_{ns}^{SO_2}(N)} f_L(N) \quad (80)$$

and because $R_c^{SO_2}$ does not have a SAI term:

$$R_c^{SO_2} = \frac{1}{G_{ns,tot}^{SO_2}} \quad (81)$$

If you run the Oslo CTM3 without the nitrate and sulphur modules, a_{sn}^{24h} should be read from a monthly model climatology.

– HNO₃ –

The surface resistance of HNO₃ is generally very small, but is reduced at cold temperatures. We follow EMEP2012, but with a minimum value of 1 s/m instead of 10:

$$R_{ns}^{HNO_3} = \max(1, -2 T_{2M}) \quad (82)$$

– Other gases –

Other gases (except CO; see below) are interpolated using conductances from O₃ and SO₂:

$$G_{ns,tot}^i = 10^{-5} H_*^i G_{ns,tot}^{SO_2} + f_0^i G_{ns,tot}^{O_3} \quad (83)$$

where H_*^i and f_0^i are taken from tables in Wesely (1989), also listed in Table 8. From these we find the surface resistance for gas i :

$$R_c^i = \frac{1}{G_{ns,tot}^i} \quad (84)$$

There is no need of doing this calculation for each land-use type, as the interpolation itself introduces uncertainties, and because there are so little data available on non-stomatal resistances, this simpler scaling is acceptable (EMEP Report 1/2003).

In Oslo CTM3, this method is applied for PAN, H₂O₂, NO₂, NO, HCHO and CH₃CHO.

– CO –

CO uptake is very small and the Oslo CTM2 parameterisation, namely a fixed deposition rate of 0.03 cm/s over forest and grass lands.

Note on stability scaling

The old deposition scheme adjusted dry deposition velocities according to stability, following:

$$v_{d,adj} = \frac{v_d}{1 + \frac{v_d z}{K_z}} \quad (85)$$

where z is the mid-point of the surface layer and K_z the eddy coefficient calculated by the boundary layer mixing routine. Physically, it is the mixing of the surface level that is reduced, and it is carried out for species using the old treatment at the end of `setdrydep`, and the unit is still [m/s].

This scaling is not used for the EMEP parameterisation, which already takes stability into account through u_* and other meteorological variables.

7.2.4 Technical description: aerosols

The sea salt (Section 16) and mineral dust (Section 15) modules have their own deposition routines. For BC/OC, sulphate and SOA, however, we use the EMEP treatment (Simpson et al., 2012). They give the dry deposition velocity v_d as

$$\frac{V_d}{u_*} = \begin{cases} a_1 & : L \geq 0 \\ a_1 F_N \left[1 + \left(\frac{-a_2}{L} \right)^{2/3} \right] & : L < 0 \end{cases} \quad (86)$$

where $F_N = 3$ for fine-nitrate and ammonium, and $F_N = 1$ for all other aerosols. Simpson et al. (2012) limit this to $1/L < -0.04 \text{ m}^{-1}$, which means that for $-25 < L < 0$ we use $L = -25$ in Eq. (86).

The parameters a_1 and a_2 are

$$a_1 = \begin{cases} 0.002 & \text{non-forest} \\ \max(0.002, 0.008 \frac{SAI}{10}) & \text{forest} \end{cases} \quad (87)$$

$$a_2 = 300 \text{ m} \quad (88)$$

In principle, a_1 could differ from dry to wet surfaces. This is not yet taken into account for sulphate, MSA, nitrate and SOA. For BC/OC, however, we have calculated our own parameters based on mean values of Oslo CTM2 for water, land and ice surfaces, as well as the annual mean friction velocity ($\overline{u_*}$):

$$a_{1,L} = \frac{V_{land}}{\overline{u_*}} \quad (89)$$

$$a_{1,W} = \frac{V_{water}}{\overline{u_*}} \quad (90)$$

$$a_{1,I} = \frac{V_{ice}}{\overline{u_*}} \quad (91)$$

The V -values are defined in the BC/OC module (Section 14) as 0.025 cm/s, with the exception of hydrophilic aerosols over wet surfaces which use 0.2 cm/s.

7.2.5 Soil uptake of CH₄

If CH₄ emissions are included (Section 8.9), a soil sink also has to be included: CH₄ is taken up in soils by microbacteria, and this process can be modelled as dry deposition. In Oslo CTM3, this requires a deposition velocity, which currently is calculated from two datasets; soil uptake in kg/s from a dataset provided by Bousquet (Section 8.9), and CH₄ mass in the surface gridboxes of T42L60 resolution, calculated during the HYMN project.

The routines taking care of this are located in the file *ch4routines.f90*.

7.2.6 Inside or outside chemistry?

There are two ways to treat deposition in the Oslo CTM3; the Oslo way and the UCI core method.

In the UCI core method, tracers are removed by deposition as a separate process in the operator split loop. This allows for better control over diagnostics.

The Oslo method is to treat dry deposition as a loss term in chemistry, along with treating emissions as source terms. You define the method you need in the user specified section of *Makefile*. This is described in Section 8; remember that this also moves emissions into chemistry. Note that e.g. mineral dust and sea salt modules have their own deposition calculations.

The two methods should be tested thoroughly against each other.

7.2.7 UCI dry deposition

It is in principle possible to use the UCI CTM deposition scheme, which is very simple, listing deposition velocities for 3 different soil types (listed in the old scavenge list *scavng55.dat*).

7.3 Uptake on aerosols

A third option for scavenging of gases is uptake on aerosols. This may involve reactions which release products back to the atmosphere, and is thus sometimes referred to as heterogeneous reactions.

Currently, there is only tropospheric uptake of N₂O₅, producing HNO₃, and uptake of HO₂ and RO₂. In the stratosphere there are a few other aerosol uptake processes.

The tropospheric uptake is in the process of being revised.

8 Emissions

Emissions can largely be divided into surface, lightning and aircraft emissions. Surface emissions can further be divided into anthropogenic, biomass burning (often distributed vertically), natural biogenic, natural oceanic and natural soil emissions.

How emissions are treated in Oslo CTM3 is explained in Section 8.1, before a short note on NO_x. How to set up different emission sets and include new sets are described in Section 8.3.

Different types of emissions are explained in the following sections.

Note that emissions are always stored with units of kg/s. When used as chemical production terms, the units are converted to molecules/cm³/s.

8.1 Emissions treatment

Emissions can be treated in two ways in the Oslo CTM3.

- Inside chemistry as a chemical source (Oslo method, Section 8.1.1).
- As a separate process (UCI method, Section 8.1.2).

The choice of approach is set in *Makefile*, by the variable `EMISDEP_TREATMENT`. The default choice is the Oslo treatment until extensive testing has been carried out.

8.1.1 Emissions in chemistry

In the traditional Oslo chemistry method, the emissions are treated as chemical source terms (and deposition as a sink). This method aims to combine several of the operator split processes in one.

One advantage of this treatment is a quasi steady state between sources and sinks, so that parts of what is emitted is also lost (when a sink is present). This method will give smoother time series, since the sources and sinks compete in the calculation.

At the moment this is the default treatment in Oslo CTM3.

8.1.2 Emissions as a process

The other approach is the UCI method (`EMISDEP_TREATMENT :=U` in *Makefile*), treating emissions as a separate process (routine `SOURCE`). Emissions are put directly into the tracer array (as mass, kg), before they are mixed in boundary layer mixing and then the chemistry is calculated. For this method, the emissions may impose a large change in the concentrations, causing a larger adjustment in the chemistry. It is important to do boundary layer mixing after emissions to reduce the artificial impact in the surface layer.

With this method it is possible to better diagnose every step of the operator split processes. This is useful for evaluating the model and its resolution (e.g. time step vs convergence).

After extensive testing is carried out, this may eventually become the default emission treatment in Oslo CTM3.

Important

Note that e.g. sea salt has separate production routines, using QSSA. This will have to be revised if you want sea salt production as a separate process (see also Section 16.2). Probably less straight-forward is to change

the mineral dust production from DEAD treatment to a separate source.

8.2 Important about NOx

NOx is treated as a family in the Oslo chemistry. Traditionally this NOx family was also transported, but since all its components are transported there is no longer need for the family to be transported, and hence not emitted.

8.3 How to set up emissions

The emissions are listed in the file *Ltracer_emis_XXX.inp*, where *XXX* is e.g. *eclipse_V5*. You will find some information at the top of the file, followed by a section with flags and data for special emissions (e.g. aircraft emissions). After this the 2D and 3D monthly emissions are listed separately.

Next, there's a section containing static fields used in the model to generate other relevant emissions, e.g. emissions that are be updated more frequently. The section is named STV for short term variation. Examples are DMS emissions, volcanic emissions and dust emissions.

Finally, there is a section for biomass burning, denoted 'BBB'.

The emission datasets are described in next Sections, however, here is a short how-to.

It is important to make sure you include all categories you need; and that sources are not covered by different datasets at the same time:

- aircraft emissions
- anthropogenic emissions
- biomass burning emissions
- lightning emissions
- natural biogenic emissions
- natural oceanic emissions
- natural soil emissions
- volcanic emissions

Some datasets are given for one year only, e.g. 2000, while others are given for different years. If you want to interpolate between the datasets, the easiest way is to include both datasets in the *Ltracer_emis_XXX.inp* and apply weightings for each dataset. E.g. for 2001 you can include 0.8 of the 2000 dataset and 0.2 of the 2005 dataset.

You should also be aware that some datasets, such as ECLIPSE, include agricultural waste burning as anthropogenic emissions, while it is also present in the GFED biomass burning datasets. You need to apply only one of these. This will be explained in the subsections of Section 8.11.

For each section in the emission list, the read-in structure is shown first, with a more detailed explanation at the bottom of the file. An example from the 2D section is shown in Table 10.

The different variables to set are described at the bottom of the file:

- **ID:** Tag referring to the format to read. When including a new set with a new structure, a new read-in code has to be included.
- **SCALE:** Scaling factor which applies for the whole dataset.
- **RES:** String describing the resolution; 1x1 for 1 degree, HLF for 0.5 degree, and ZP1 for 0.1 degree.
- **MONTH:** The month the dataset applies for. 99 is all months.
- **YEAR:** The year the dataset applies for. 9999 is all years.
- **CAT:** The category for the dataset. This is used for diagnostics only, summing up emissions for each category.
- **TYPE:** Defines whether the field should be scaled with area or not. 0 when field is not per area, 1 when field is 1/cm² and 2 when field is 1/m².
- **UNIT:** To define the unit of the dataset, so correct scaling is applied in the emission routines. If per area, it is combined with non-zero TYPE. 1 for kg/s, 2 for moelc/s, 3 for kg/y, and 4 for kg/month.
- **DIURN:** Flags a dataset for diurnal variation. See Section 8.4.2 for more. 0 for no diurnal variation, 1 for RETRO local hour variations, 2 for +50 % from 8 am to 7 pm and -50 % from 8 pm to 7 am. DIURN=3: Scaling with *T* and daylight, DIURN=4: Scaling with daylight, DIURN=5: Heating degree day (HDD) scaling.
- **VERT:** Flags whether 2D dataset should be distributed vertically on the lowermost model levels (altitudes about 0-16m/16-41m/41-77m/77-128m). Several options are available, although none are documented yet. They should be documented as soon as possible. VERT=1: 0.25/0.125/0.125/0.5 (typical power/industrial combustion), VERT=2: 0.6/0.2/0.2/0.0 (typical residential heating), VERT=3: 0.3/0.4/0.3/0.0 (typical ship emissions).
- **DATASET_NAME:** The name of the dataset on file, needed for e.g. netCDF files.
- **SCENYEAR:** The year to extract data for – used for read-ins where the file contains several years of data. If the file only contain data for a specific year, this is not used.
- **SPECIES:** the component for which the dataset is to be applied. If species differ from what the dataset applies for, a scaling factor may be needed to account for differences in molecular masses (SCALING).
- **SCALING:** Scaling factor for SPECIES, for the given dataset. Use this for taking different molecular weights into account, e.g. as shown for NO in Table 10.

Important: The scaling of components must take into account differences in molecular weights. However, if the emission dataset is given in molecules, such a scaling should *not* be included. See the two NO/NO₂ examples in Table 10.

8.4 Emission datasets

As already mentioned, there are several emission inventories available, and most are listed in the directory *tables/EMISSION_LISTS*. Usually, the natural and anthropogenic emissions are separated into different datasets. E.g. natural biogenic, oceanic and soil emissions may be taken from POET (Granier et al., 2005;

Table 10: Structure of the emission file *Ltracer_emis_***.inp*. Note how NO and NO₂ are scaled when data is given as kg or molecules.

```

-2D-- 2D emissions -----
filename / description (See detailed description below)
  ID      SCALE      RES MONTH YEAR  CAT TYPE UNIT DIURN VERT DATASET_NAME SCENYEAR
  SPECIES SCALING ('xxx' to close dataset)
'/full_path/some_emission_file_of_anthropogenic_CO_2000_0.5x0.5.nc'
  601     1.0000d+00  HLF   99  9999  AGR   2    0    1    0  'emiss_agr'  0000
  CO  1.d0
  xxx 0 To close this data set
'/full_path/some_emission_file_of_anthropogenic_NO_2000_0.5x0.5.nc'
  601     1.0000d+00  HLF   99  9999  AGR   2    0    1    0  'emiss_agr'  0000
  NO  0.96d0
  NO2 0.0613333333d0      # NO on file: 0.04*46/30
  xxx 0 To close this data set
'/work/projects/cicero/ctm_input/EMIS/RETROEMIS_NEW/soils.nox.nc' 0000
  601     1.0000d+00  1x1   99  9999  BIO   1    1    0    0  'bio'
  NO  0.96d0      # molecules on file, no need to scale NO2/NO
  NO2 0.04d0
  xxx 0 To close this data set

```

Olivier et al., 2003). Biogenic emissions may rather be taken from more recent MEGAN datasets, but note that MEGAN does not comprise oceanic emissions, nor soil emissions of NO_x. Recently, a newer MEGAN dataset has become available, the so-called MEGAN-MACC (Sindelarova et al., 2014). Anthropogenic emission datasets are e.g. CEDS, RETRO, Lamarque et al. (2010), EDGARv4.2 or ECLIPSE.

You specify which emission datasets to include in the emission list *Ltracer_emis_***.inp*. See Section 8.3 for a description on this.

All these emissions are read by the routine `emis_input` in *emissions_oslo.f90*. Any dataset can in principle be used, although you may have to include new read-in routines.

There are currently no studies on which dataset is the best, and how they affect the model results. Generally, the newer datasets should be better because they are more up-to-date. However, some datasets lack seasonal variation, which could be important for your study.

Note that some specific components need more specific/hard-coded parameterisations, like forest fires (Section 8.5) and aircraft emissions (Section 8.7). Such emissions are updated by `update_emis` in *emissions_oslo.f90*.

8.4.1 Monthly & annual emissions

The monthly and annual emissions can be 2D or 3D. 2D fields are stored in the array `E2DS(IPAR,JP,AR,NE2DS,ETPAR)`, where `NE2DS` is usually 1, but can be 6 if you want moments included (described below). `ETPAR` is the max number of tables, and there is a counter for the actual number of tables used, `NE2TBL`.

If you have emissions as a separate process (UCI method), and if the emissions are on a higher resolution than the

model resolution and you want higher accuracy for where emissions are put out, it is possible to include moments in the 2D emissions. To do this you have to hard-code `NE2DS=6` in *cmn_size.F90*. This is only for experienced users. It is probably wise to leave out moments for horizontal resolutions higher than T159.

When treating emissions inside chemistry, the moments *cannot* be included (`NE2DS=1`).

There can be max `E3PAR` 3D fields, and they are given in `E3DSNEW(LP,AR,JP,AR,E3PAR)`, which is changed from the UCI core due to striding in the original `E3DS(IP,AR,JP,AR,E3PAR)`. The counter for used fields is `NE3TBL`.

Forest fires are treated separately (Section 8.5) and there are also some other short term variations based on monthly or annual data (Section 8.4.4).

The Oslo CTM3 should in general be modified to read monthly emissions each month, to save memory requirements.

8.4.2 Diurnal scaling

Diurnal variations can be imposed on the 2D monthly/annual datasets. This is done by setting the `DIURN` flag in *Ltracer_emis_***.inp*. The `DIURN` flag is described below, and *Ltracer_emis_***.inp* in Section 8.3).

The `DIURN` can either scale to local hour or by a 2D field. Local hour scaling emits more during certain hours than at other, presently with an hourly temporal resolution. Scaling the dataset to a 2D field usually means that it is scaled by meteorological properties such as temperature. These scalings need reference fields, e.g. on monthly basis.

Available diurnal variations

When the flag `DIURN` is set for a dataset listed in *Ltracer_emis_***.inp*, a diurnal variation is applied to

the dataset. Currently the possibilities are

- **DIURN=0:** No diurnal variation.
- **DIURN=1:** RETRO variations (TNO²).
- **DIURN=2:** +50 % from 8 am to 7 pm and -50 % from 8 pm to 7 am.
- **DIURN=3:** Scaling with T and daylight.
- **DIURN=4:** Scaling with daylight.
- **DIURN=5:** Heating degree day (HDD) scaling.

If you need other scalings, inclusion of new ones should be rather straightforward once you know the system. **DIURN=1** and **DIURN=2** can in principle be set up to work on 3D fields, but is currently not used.

Local hour scalings

These are found in the variable **E2LocHourSCALE** and of size 24, **NECAT**, **NE2LocHourVARS** and are defined in *cmn_oslo.f90* and set in *emisutls_oslo.f90*, routine **set_diurnal_scalings**

RETRO variations

DIURN=1 sets the RETRO variations (TNO³). There is one scaling per category.

Note that these work for pre-defined categories.

+50 % –50 %

DIURN=2 sets +50 % from 8 am to 7 pm and -50 % from 8 pm to 7 am.

Variations with T and daylight

Some species, typically naturally emitted isoprene and monoterpenes, are emitted only during daytime, whereas the emission files are usually monthly or annual means. In Oslo CTM3 we have the possibility to scale surface emissions so that they are emitted only during daytime. In addition, it is possible to scale according to temperature, i.e. daytime temperature. In other words, these are more complex diurnal scalings than the local hour predefined scaling.

Monthly-based daylight scaling

The daylight scaling is a 2D field of the fraction of daylight hours during the month, which we denote f_{day} . It is possible to modify this to a daily basis, but the monthly basis was chosen to match monthly emissions.

For each hour we check if there is daylight, and scale up the emissions E :

$$E_{day} = E / f_{day} \quad (92)$$

During night there is consequently no emissions, except that when there is polar night, i.e. no daylight during a day, we set $f_{day} = 1$. This is of minor importance for species such as isoprene and monoterpenes, which should have very small emissions during the polar night. You set this option by **DIURN=4** in the emission list.

Monthly-based day-temperature scaling

Another surface scaling field is based on temperature and daylight for the years 1997–2010 using our T42L60 meteorological data (ECMWF IFS cycle 36r1).

This method is based upon Guenther et al. (1995), who described the effect of temperature on emissions of VOCs.

²Nederlandse Organisatie voor Toegepast Natuurwetenschappelijk Onderzoek

³Nederlandse Organisatie voor Toegepast Natuurwetenschappelijk Onderzoek

They found that the emissions E could be described by variation around a standard emission E_s at a standard temperature T_s :

$$E = E_s f_T \quad (93)$$

$$f_T = \frac{\exp\left(\frac{C_1(T-T_s)}{RT_s T}\right)}{1 + \exp\left(\frac{C_2(T-T_m)}{RT_s T}\right)} \quad (94)$$

Three empirical constants are used here: $T_m = 314$ K, $C_1 = 95000$ and $C_2 = 230000$.

Using f_T in Eq. (94), a standard temperature $T_s = 303$ K, and 3-hourly surface temperatures from our 1997–2010 meteorology, we have computed climatological monthly means of f_T , namely f_{Tclim} . When applied to a monthly emission inventory, we calculate E_s from Eq. (93), using f_{Tclim} . Since E_s is the climatological emissions at the standard temperature, we can each hour in the model scale with f_T using T at that time step.

Note that this method is also taking only daylight into account, as described above, except in polar night, where temperature scaling is carried out using temperatures for the whole day/night. You set this option by **DIURN=3** in the emission list.

Heating degree day (HDD) scaling

HDD is defined as a difference temperature in Kelvin:

$$HDD = \max(0, 288.15 - T_{sfc}) \quad (95)$$

Weighting the surface temperature T_{sfc} by the time steps of the meteorological data (3 hr), HDD has been summed up on monthly and annual basis, giving the fraction of monthly to annual HDD . This is done for specific years. To be applied monthly on annual data of units kg/s, this fraction has to be converted to a scaling by multiplying with 12; the sum of the 12 scalings for a grid box should not be 1, but 12, because we are scaling up or down annual mean kg/s and applying it for different months.

This is so far only set up on a monthly basis, but could in principle be updated every meteorological time step. Stohl et al. (2013), however, found that using a monthly variation was a good approximation.

8.4.3 Vertical distribution of 2D emissions

For 2D emission datasets, it is possible to distribute the emissions into four of the lowermost model layers. These layers roughly cover surface–16 m, 16–41 m, 41–77 m and 77–128 m (the actual thickness depends on surface pressure, temperature and specific humidity, see Appendix C.2).

The distributions are not documented yet, but were used in Oslo CTM2:

- **VERB=0:** All in surface layer.
- **VERB=1:** 0.25/0.125/0.125/0.5, typical for power and industrial combustion.
- **VERB=2:** 0.6/0.2/0.2/0.0, typical for residential heating.
- **VERB=3:** 0.3/0.4/0.3/0.0, typical for ships.

Defined in *cmn_oslo.f90*, there are **NE2vertVARS** distributions, and the distributions are stored in the variable **E2vertSCALE**.

8.4.4 Short term variations

Some emissions are not given on monthly or annual basis, but depend strongly on e.g. wind or temperature. Examples are DMS from ocean and sea spray. Organic matter from sea spray is also difficult to retrieve from a separate monthly dataset.

The STV section of the emission list allows inclusion of some of these datasets.

DMS from ocean

DMS is emitted continuously from ocean water, and those emissions are parameterized using climatological concentrations of DMS for each month, combined with winds from the meteorological data. See Section 13.1 for more.

The concentration is read into `DMSseaconc`, and has units of nM (nanoMolar), i.e. nmole/L. The units are then converted to kg/m and multiplied with a velocity based on the wind speed. This is carried out in the `SOURCE` routine or in `emis4chem_oslo` when using emissions as production terms in chemistry.

Organic matter from ocean

The emission of organic matter from ocean follows Gantt et al. (2015), based on chlorophyll A and sea spray.

Sea spray is taken from the sea salt module if it is included. Several schemes are available, as described in Section 16.1, using the flag `SeaSaltScheme`. If the sea salt module is not included, this sea spray is calculated by the organic matter emission routine, using its own flag `SeaSaltScheme`.

Oslo CTM3 use Chlorophyll A from MODIS, where monthly data for the years 2003–2014 are available. A climatology for the same years have been generated, and the user specifies whether to use the climatology or not in the emission list.

The MODIS monthly mean data are fetched from <http://oceandata.sci.gsfc.nasa.gov/MODISA/Binned/Monthly/> where the files `A*L3b_MO_CHL.main.bz2` are retrieved and unzipped. Files are converted to netcdf using IDL program `read_chla.pro` (located in the utilities directory) which applies the program `readl3bin.pro`. Recently, the MODIS files are available directly on netCDF format, which should rather be used.

The climatology is generated from netCDF files using the IDL program `chla_avg.pro`.

DUST emissions

Emissions of mineral dust should be defined in the STV section, as explained in Section 15.3.1.

8.5 Forest fires emissions

Several species are affected by forest fires, and emissions may be updated more frequently than each month. Due to this, the forest fires need to be coded separately.

It is recommended to use daily GFEDv4 emissions, distributed in the boundary layer, using the format code 572 in the emission list, i.e. daily emissions. If daily emis-

sions are not available (years prior to 2003), you should use monthly emissions (code 571). Some other options for GFEDv4 are described below.

The code defines `FF_TYPE`, while the year defines `FF_YEAR` and the path defines `FF_PATH`. See Table 11.

A diurnal cycle is further added, according to Roberts et al. (2009), putting increasing daytime emissions by 90 % (7–19 local hours) and reducing nighttime emissions to 10 %.

An alternative dataset to GFEDv4 is monthly CEDS biomass burning, which is set up with the old vertical profile (code 568) and the altitude weighted boundary layer profile (code 574).

You find the inputs to the emission list in `Ltracer_emis_biomassburning.dat` in `EMISSION_LISTS`. The list includes scaling factors for different species.

Historically, the biomass burning emissions have been distributed in the vertical by a distribution from RETRO. This should be left behind, as it is not very physical. We rather distribute the emissions within the boundary layer. The old profile probably put too much above the boundary layer, so with the new method, over-shooting is reduced.

If over-shooting is needed, you should make a distribution on the emission strength in the emission dataset, and for the strongest sources (e.g. defined by 90-percentile) select the grid boxes where over-shooting may occur.

Two test options are included, distributing emissions according to air mass in the boundary layer (air mass weighted), namely code 570 (`FF_TYPE=6`, monthly emissions) and 571 (`FF_TYPE=7`, daily emissions). These put emissions a bit closer to the surface than the altitude-weighted profile.

The read-in is called from `update_emis` (in `emissions_oslo.f90`), and there you can see which routines are called for the different choices.

Note that the daily fractions require the monthly field to be read every day (for the future, consider storing it). The daily fractions have to be applied prior to regridding.

The species emitted are listed in the BBB section of the emission list, and are typically CO, NO_x, hydrocarbons, NH₃, SO₂ and black and organic carbon. The emissions are distributed vertically based on RETRO vertical distribution.

The number of components treated is given as `NEFIR`, with an upper limit of `EPAR_FIR`. Their transport numbers are given in `ECOMP_FIR(EPAR_FIR)` and emissions are stored in the array `EMIS_FIR` with dimension `(EPAR_FIR_LM, EPAR_FIR, IDBLK, JDBLK, MPBLK)`. The array structure makes it easy to use with very little striding.

Note that the read-in from file is placed outside the parallel region of the model, because the interpolation is parallelized.

Other variables used for determining species and file names, which are read from emission list, are:

- `FF_CNAMES`: Emitted component.

Table 11: Biomass burning variables used by the Oslo CTM3. Default `FF_TYPE` is 9 (or 8 if daily fractions are not available).

| Variable | Option | Description |
|----------------------|--------|--|
| <code>FF_TYPE</code> | 4 | GFEDv4 monthly (code 567) |
| | 5 | CEDS monthly (code 568) |
| | 51 | CEDS monthly (code 574), distributed according to model level thickness in the boundary layer. |
| | 6 | GFEDv4 monthly (code 569), distributed according to air mass in the boundary layer. |
| | 7 | GFEDv4 daily (code 570), distributed according to air mass in the boundary layer. |
| | 8 | GFEDv4 monthly (code 571), distributed according to model level thickness in the boundary layer. |
| | 9 | GFEDv4 daily (code 572), distributed according to model level thickness in the boundary layer. DEFAULT. |
| <code>FF_YEAR</code> | 9999 | Use current meteorological year (<code>MYEAR</code>), or specify which year to use. |
| <code>FF_PATH</code> | | Path to where emissions are. |

- `FF_BNAMES`: Component name used in file name.
- `FF_SCALE`: Scaling factor.
- `FF_PARTITIONS`: Partition factors (GFED only).

Forest fire partitions

It is possible to turn off specific partitions of the GFEDv4 data. There are six partitions:

- agriculture
- deforestation
- forest
- peat
- savanna
- woodland

The turning off is done by hard-coding the flags `partitions` in the routine `gfed4_rd_*`, the read-in located in `emisutils_oslo.f90`.

One example where you have to do this, is for ECLIPSE emissions of black carbon, where you have to turn off agricultural waste burning (AWB), because it is included in the ECLIPSE dataset. See Section 14 for more.

8.6 Biogenic emissions: MEGAN

The emission model MEGAN, version 2.10 (Guenther et al., 2012), is included in the Oslo CTM3. You turn it on by including it in the emission list (STV section), as in Table 12.

Turn off other biogenic emissions! Make sure that other biogenic emission datasets are not included in the 2D section of the emission list. Also NO_x from soil emissions should be turned off.

The MEGAN model uses leaf area index (LAI) and roughness length (Z_{0I}). See Section 20.6 and Section 20.7, respectively.

Here will follow a description of MEGAN and the changes done for Oslo CTM3.

8.6.1 Modifications to MEGAN code

The MEGANv2.10 code has been adopted to Oslo CTM3, in other words stripped and cleaned up to fit the Oslo CTM3 structure. Input to MEGAN is through `megan_tables.dat`, found in the `tables/` directory.

Here is a list of the tables (in appearing order):

1. Megan original species (20 of them). Note that soil NO_x is included, even if it is not described by (Guenther et al., 2012).
2. Canopy types, or plant function types (PFTs). There are 16 of these, listed in Table 13, and stored in the variable `landSurfTypeFrac`. See also Section 20.5.
3. Canopy Characteristics, listed in Table 13.
4. Emission factors for the 20 MEGAN species for each canopy type. This is Table 2 in Guenther et al. (2012).
5. Emission factors for each speciated species (151 of those). In the MEGAN original, these should sum up to 1 for each of the 20 species. Note that while MEGAN originally does not take molecular masses into account, we have to do this at least for NO and NO₂. This is explained in the text.

Molecular weight: MEGAN does take into account possible differences in molecular weights of the 20 species when speciation to 150 species is done. This means that it calculates a total mass for each of the 20 species, and then distributes the masses on each component.

This may be problematic when species of very different molecular weights are lumped together. E.g. if we want to emit NO as 4% NO₂ or some other fraction as NH₃, it would distribute the total mass of NO, not considering that NH₃ is lighter or NO₂ heavier.

Taking the molecular weight of the 20-species into account would solve this, but is clearly not what was intended in MEGAN.

Table 12: Turn on the online MEGAN biogenic emissions by including this in the STV section of the emission list.

```
-STV- Used for short time variations; only one species per field -----
'Indata_CTM3/MEGAN/'
  557    1.00000d+00  HLF    99  9999  BIO    0   -1    0   '---'  9999
  ---    #This section defines the use of MEGAN and sets path to MEGAN datasets
```

NO, NO₂ and NH₃: I have therefore kept the MEGAN method, but for NO the speciation factors have to take into account the difference in molecular weights. These are thus scaled so that 4% of NO is emitted as NO₂. The total atmospheric source of NO_x is 6 Tg(N) from soil, based on towards a mechanistic model of global soil nitric oxide emissions: implementation and space based constraints (2012), assuming a total source of 7.5 Tg(N) combined with canopy uptake of 20%. Inclusion of NO₂ makes it 151 speciated species in total.

Emission factors for the 20-species NO have been increased to match WRF factors. This increase is more than conversion from N to NO. This gave an annual total of 4.93 Tg(NO) for year 2000. We use the speciated factors to scale up to 12.85 Tg(NO)/year (i.e. 6 Tg(N)/year). Putting 4% on NO₂, we get speciated factors for NO = 2.50 and NO₂ = 0.16 (taking conversion of NO to NO₂ into account).

NH₃ is also emitted from soils, and is scaled to match GEIA totals of 7.32 Tg(NH₃) (4.36 from crops and 2.96 as natural vegetation). Our value of 4.93 Tg(NO)/year is used to estimate the NH₃ speciation factor, i.e. 2.620. Since MEGAN operates on mass, this scale will get us the mass we need for NH₃ (unlike NO₂ where molecular masses are taken into account, converting NO to NO₂ on the way into the atmosphere).

The sum of speciation factors for nitrogen components is thus larger than one.

Global scaling factor: The global scaling factor *Cce* is set to 0.483, to match the total isoprene emissions in MEGAN-MACC (Sindelarova et al., 2014) for year 2000 (i.e. 572 Tg/yr), using 1982–1998 climatology of LAI and *z0*. The scaling factor was originally 0.56 in the MEGAN code, whereas e.g. CLM uses 0.4 (Guenther et al., 2012).

DI initialised: The Palmer severity draught index (DI) was never initialised, and is set to zero. In the original MEGAN code it was allocated and that supposedly set it to zero also.

STRESS components: Some of the 150 species (e.g. ethene) were assigned to 20-component number 19, but named 'STRESS', which is component 20. This was corrected, giving about 50% lower emissions due to the different emission factors.

8.6.2 MEGAN total emissions

The emissions of Oslo CTM3 species coming from MEGAN are diagnosed following the BUDGETS calendar, and put in files *emis_accumulated_3d_megan_*.nc*, similar to regular emission tendencies.

Table 14 lists the Oslo CTM3 MEGAN emissions for year 2016, and although a different year than listed in Guenther et al. (2012), the values match well. Note that a higher isoprene emission is found for 2016, about 80 Tg/yr more than for year 2000.

8.7 Aircraft emissions

Aircraft emission routines are located in *emissions_aircraft.f90*. You define which scenario (**AirScen**) to use in *Ltracer_emis_*.inp*, along with the path to aircraft emissions (**AirEmisPath**). If you add new emissions, the read-in will have to be updated. As for other gaseous species, the emissions are added to the global emission arrays.

There is no plume chemistry yet, as we have left the NILU plume parameterisation behind, but this can eventually be included.

Aircraft emissions of H₂O are treated as a separate tracer, since H₂O is not transported in the troposphere, and depending on your setup, maybe not in the stratosphere. This separate aircraft H₂O tracer is given the tracer number 148, and must be transported. It is removed below 400 hPa according to Danilin et al. (1998), by assuming a lifetime of 1 hour.

8.8 Lightning emissions

Lightning is a major contributor to NO_x in the atmosphere, assumed to amount to 5 ± 3 Tg(N)/year (Shumann and Huntrieser, 2007). As will be described below, we use a climatological value of ~ 5 Tg(N)/year, i.e. the emissions will vary somewhat from year to year due to different meteorologies.

To properly parameterise lightning emissions, a horizontal (geographical) distribution of lightning strikes must be used, and then a vertical distribution must be applied.

In general, lightning flash rates in Oslo CTM3 are connected to the horizontal distribution of convection, thus depending on the meteorological dataset you use. To convert to observed flash rates we need scaling factors, and these will differ for different meteorological data (also for different cycles or resolutions). A step-by-step recipe on how to calculate these scaling factors is explained in Section 8.8.7, but first you should understand the horizontal and vertical distributions.

The horizontal distribution of lightning NO_x (L-NO_x) was updated in 2011 by Chris D. Holmes at UCI, and was documented in Søvde et al. (2012). However, it was locked to the T42 resolution, and had to be updated in

Table 13: Canopy types (PFTs) and canopy characteristics used in MEGAN.

| # | Canopy type |
|----|-------------------------------------|
| 1 | Needleaf evergreen temperate tree |
| 2 | Needleaf evergreen boreal tree |
| 3 | Needleaf deciduous boreal tree |
| 4 | Broadleaf evergreen tropical tree |
| 5 | Broadleaf evergreen temperate tree |
| 6 | Broadleaf deciduous tropical tree |
| 7 | Broadleaf deciduous temperate tree |
| 8 | Broadleaf deciduous boreal tree |
| 9 | Broadleaf evergreen temperate shrub |
| 10 | Broadleaf deciduous temperate shrub |
| 11 | Broadleaf deciduous boreal shrub |
| 12 | Cool/Arctic C3 grass |
| 13 | C3 grass (cool) |
| 14 | C4 grass (warm) |
| 15 | Crop 1 (Corn) |
| 16 | Crop 2 (Other crops) |

| # | Canopy characteristics |
|----|--|
| 1 | canopy depth (height above ground is canopy height minus canopy depth) |
| 2 | leaf width |
| 3 | leaf length |
| 4 | canopy height |
| 5 | scattering coefficient for PPFD |
| 6 | scattering coefficient for near IR |
| 7 | reflection coefficient for diffuse PPFD |
| 8 | reflection coefficient for diffuse near IR |
| 9 | clustering coefficient (accounts for leaf clumping influence on mean projected leaf area in the direction of the suns beam) use 0.85 for default, corn=0.4-0.9; Pine=0.6-1.0; oak=0.53-0.67; tropical rainforest=1.1 |
| 10 | leaf IR emissivity |
| 11 | leaf stomata and cuticle factor: 1=hyposomatous, 2=amphistomatous, 1.25=hyposomatous but with some transpiration through cuticle |
| 12 | daytime temperature lapse rate (K m-1) |
| 13 | nighttime temperature lapse rate (K m-1) |
| 14 | warm (>283K) canopy total humidity change (Pa) |
| 15 | cool (>= 283K) canopy total humidity change (Pa) |
| 16 | normalized canopy depth where wind is negligible |
| 17 | canopy transparency (included in MEGAN3) |

order to properly use higher resolutions. The current version is documented below as OAS2015 (Section 8.8.1), while the GMD version is documented as GMD2012 (Section 8.8.2). In addition, I have listed here also the 2015 version of UCI (UCI2015) and another method (AP2002).

Table 14: MEGAN annual emissions in Oslo CTM3, for year 2016.

| Species | Tg/yr |
|---|--------|
| Isoprene | 649.06 |
| CO | 107.45 |
| Formaldehyde (CH ₂ O) | 5.71 |
| Ethene (C ₂ H ₄) | 33.76 |
| Propene (C ₃ H ₆) | 15.24 |
| Acetone | 39.45 |
| α -pinene | 65.84 |
| β -pinene | 20.24 |
| Limonene | 11.61 |
| Ocimene | 17.32 |
| D3carene | 8.07 |
| Myrcene | 8.60 |
| Sabinene | 9.21 |
| Terpinolene | 1.21 |
| Terpinene | 2.31 |
| Terpene Alcohol | 4.56 |
| Sesquiterpenes | 24.85 |
| Terpinene-ketone | 3.23 |
| Toluene++ (Tolmatic) | 1.75 |
| Acetaldehyde (CH ₃ CHO) | 28.19 |
| Dimethylbenzene++ (C ₆ H ₁₀) | 1.63 |
| Dimethylsulfide (DMS) | 1.59 |
| NO | 14.31 |
| NO ₂ | 0.92 |
| NH ₃ | 8.28 |
| Total VOC+CO | 1060.9 |

8.8.1 Horizontal distribution – OAS2015

The Price et al. (1997) equations for flash rates over land and ocean are the basis for Oslo CTM3 L-NOx:

$$f(\vec{x}, t) = \begin{cases} f_L(\vec{x}, t) = s_L P_L(\vec{x}, t) & \text{over land} \\ f_O(\vec{x}, t) = s_O P_O(\vec{x}, t) & \text{over ocean} \end{cases} \quad (96)$$

where P_L and P_O are the Price et al. (1997) equations for a given location \vec{x} and time t , but *without* scaling factors. s_L and s_O are scaling factors, however, the Price et al. (1997) scaling factors will most likely not be suitable when using the global meteorological fields in the model. Therefore, we generate our own scaling factors, so that the flash rates calculated from meteorological data match what is observed. These will be described below. P_L and P_O are:

$$\begin{aligned} P_L(\vec{x}, t) &= H(\vec{x}, t)^{4.92} & \text{over land} \\ P_O(\vec{x}, t) &= H(\vec{x}, t)^{1.73} & \text{over ocean} \end{aligned} \quad (97)$$

H is the cloud top height (km), which we represent by the height of the uppermost grid box having convective updraft mass flux coming into it.

Scaling factors

After P_L and P_O are calculated, they need to be scaled to match observations. I.e. we need to find s_L and s_O .

In this process, we also use the scaling factors to change units from flashes per minute (as in Price et al., 1997) to annual fraction of flashes per second (the reason will become evident in the next paragraphs).

Modelled total annual unscaled flashes for land and ocean, respectively, are then

$$\begin{aligned} f_{tot,L} &= \sum_{\vec{x},t} P_L \Delta t \\ f_{tot,O} &= \sum_{\vec{x},t} P_O \Delta t \end{aligned} \quad (98)$$

where Δt is the model time step, which for Oslo CTM3 means the meteorological time step.

In other words, $P_L \cdot f_{tot,L} \cdot \Delta t$ through the year sums up to 1 and $P_O \cdot f_{tot,O} \cdot \Delta t$ through the year sums up to 1.

Taking the observed fraction of ocean/land flashes into account, we get total scaling factors:

$$s_L = \frac{\frac{f_{L,obs}}{f_{O,obs} + f_{L,obs}}}{f_{tot,L}} \quad (99)$$

$$s_O = \frac{\frac{f_{O,obs}}{f_{O,obs} + f_{L,obs}}}{f_{tot,O}} \quad (100)$$

For each time step, we can now calculate P_O and P_L , and multiply them with s_O and s_L , respectively, to get the annual fraction of flashes per second. Multiply by the time step and climatological annual emission (e.g. 5 Tg(N)/year) and we have the amount emitted during the time step, over land and ocean separately.

Because a climatological value is assumed for the emission (e.g. 5 Tg(N)/year), the scaling factors should also be generated for several years, to make climatological scaling factors.

Scaling factors for IFS cy36r1

For IFS cy36r1, the scaling factors are calculated using T42L60 meteorology, years 1997–2010, to get a climatological mean. For T159L60 resolution, only one year (2007) is calculated and used together with the same year from T42L60, to scale the T42L60 climatological factors.

Scaling factors for OpenIFS cy38r1

OpenIFS cy38r1 is only generated in T159L60, and the scaling factors are calculated as a mean of 1995–2005. When combining grid boxes 2×2 , only the year 2005 has been used.

Observed flash rates are taken from Cecil et al. (2014), where the average flash rate over land is 36.9 fl s^{-1} and 9.1 fl s^{-1} over ocean, using the HRAC dataset (LISOT-DHRAC, 2014). A climatological flash rate of 46 s^{-1} implies an average production rate of 3.45 kg(N) per flash, or 246 mol/flash. An IDL program calculating these values is given by *lightning_lisotd.pro* in the IDL utilities.

Flash filter criteria

The challenge is to sort out which convective plumes that produce lightning. If no filtering is carried out, small flash rates can be found even in shallow convection. Based on some of the UCI2015 method and also my own testing, these are the best criteria I have found:

- Convective mass flux is filtered before use: If several intervals of fluxes are found, only the thickest interval is used. Intervals of one or two layers are disregarded.
- Convective mass flux below model layer 12 (about 1500 m or 850 hPa) is disregarded to filter away some shallow convection.
- Convective mass flux must reach at least 500 hPa.

- Entrainment into updrafts must be non-zero above 500 hPa.
- Maximum temperature in the cloud must be higher than 270.5 K.
- Minimum temperature in the cloud must be lower than 243 K.

Typically, a cloud needs both liquid and ice phase particles to produce lightning, so it is usually assumed that minimum cloud/updraft temperature must be lower than 233 K and maximum temperature must be higher than 273 K. To allow for some uncertainty around this, we include two scaling factors taking the temperature into account.

- The first considers minimum temperature, linearly increasing from 0 at 243 K to 1 at 233 K.
- The second considers maximum temperature, linearly increasing from 0 at 270.5 K to 1 at 280.5 K.

Note

As will be described next, GMD2012 use cloud fraction to make grid averages. However, cloud fraction is an instant meteorological field, while convective mass flux is accumulated. To combine them is inconsistent, since cloud fraction may be zero even if there were convective flux during the accumulated period. Hence this approach cannot be used.

8.8.2 Horizontal distribution – GMD2012

The GMD2012 L-NOx method documented by Søyde et al. (2012) uses the Price and Rind (1992) equations and measurements by Optical Transient Detector (OTD, Christian et al. (1999a)) and Lightning Imaging Sensor (LIS, Christian et al. (1999b)). The difference to the OAS2015 scheme is the filtering of convective instances producing lightning.

- There must be convective flux in the grid box column.
- The grid box average updraft velocity at ~ 850 hPa must be larger than 0.01 m s^{-1} .
- The surface temperature must be higher than 273 K while cloud top temperature must be lower than 233 K.

In addition, the cloud fraction was used. Convective vertical fluxes and the clouds that contain them occupy a small fraction of the horizontal area of a model grid square. Therefore, lightning also occupies a small fraction, a , of the model grid area. The grid-averaged lightning flash rate (\bar{f}) is then

$$\bar{f}(\vec{x}, t) = a(\vec{x}, t) f(\vec{x}, t). \quad (101)$$

where a , the area fraction experiencing lightning, is estimated as a weighted average of the cloud fractions in the column:

$$a(\vec{x}, t) = \frac{\sum_{l=1}^{l_t} f_{c,l} w_l}{\sum_{l=1}^{l_t} w_l} \quad (102)$$

Here, $f_{c,l}$ is the cloudy fraction at level l , w_l is the wet convective mass flux at level l , and l_t is the model level at the cloud top.

The observed flash rate values used here was 35 s^{-1} for land and 11 s^{-1} for ocean, as given by OTD-LIS observations during 1998–2005.

The grid box average flash rates are next constrained to match the climatological averages of 35 s^{-1} for land and 11 s^{-1} for ocean, as given by OTD-LIS observations during 1998–2005. This is done by scaling factors β_l and β_o for land and ocean, respectively, which in Oslo CTM3 also converts units from 1/min to 1/s. The final scaled box average flash rate is:

$$\bar{f}_{scaled}(\vec{x}, t) = \begin{cases} \beta_l \bar{f}(\vec{x}, t) & \text{over land} \\ \beta_o \bar{f}(\vec{x}, t) & \text{over ocean} \end{cases} \quad (103)$$

The average flash frequencies for our meteorological data 1999–2009 (ECMWF cycle 36r1, resolution T42L60), imply that $\beta_l = 6$ and $\beta_o = 210$. Søvde et al. (2012) presented the factors $\beta_l = 0.10$ and $\beta_o = 3.50$, but these were calculated using the original units of the Price and Rind (1992) equations (flashes/minute) and were therefore a factor 1/60 smaller.

Compared to the Price and Rind (1992) coefficients, the gridbox average flash rates are thus scaled up by about 6 over land and 200 over ocean to match observed flash rates.

As for the OAS2015 method, scaling factors need to be generated, thereby converting to fraction of annual flashes.

8.8.3 Horizontal distribution – AP2002

There are other possible parameterisation, e.g. Allen and Pickering (2002), where the cloud-to-ground (CG) flash frequency (LF_{cg}) is calculated from the mass flux (M) at 440 hPa. Hence, the convective plumes must reach 440 hPa, and the equation is

$$LF_{cg} = \frac{A}{A30} (a + bM + cM^2 + dM^3 + eM^4) \quad (104)$$

where the coefficients a – e are different for land and water, and:

$$0 < M < 9.6 \text{ kg}/(\text{m}^2 \text{ min}) \quad (105)$$

A is the grid box area, while $A30$ is grid box area at 30 degrees latitude (actually it was the area of a specific size, but this will be of no consequence since we scale the flash rates to match observations).

To account for intra-cloud lightning, CG fraction can be found from the cold-cloud thickness (ΔZ , Price and Rind, 1993), i.e. the depth (km) of the cloud above the freezing level. In the model, it is calculated between cloud top and the midpoint of the highest layer where the temperature exceeds 273 K.

$$f_{CG} = \frac{1}{A\Delta z^4 B\Delta z^3 + C\Delta z^2 + D\Delta z + E + 1} \quad (106)$$

In Eq. (106) it is assumed that Δz is never smaller than 5.5 km. In addition, if $\Delta z > 14$ km, f_{CG} is set to 0.02, acting as an asymptotical value. $A = 0.021$, $B = -0.648$, $C = 7.493$, $D = -36.54$, $E = 63.09$.

The total flash rate for this scheme is then:

$$f = \frac{LF_{CG}}{f_{CG}} \quad (107)$$

This method has been briefly tested in Oslo CTM3, but I found the seasonal variation of globally averaged flash

rate to misplace when minimum and maximum occur, and also it was very noisy. While the annual horizontal flash rate distribution was not too bad, the variation was also very large. This method would therefore probably not be used, but it is included in the source code anyway.

8.8.4 Horizontal distribution – UCI2015

The 2015 method of UCI is explained in the lightning source code and will not be mentioned here. I have decided not to use it, because it has a very weak flash rate seasonal cycle, and the distribution is not documented anywhere. It is also not very physical when it comes to filtering the convective lightning events.

8.8.5 Horizontal distribution – other

The parameterisation described by Grewe et al. (2001) could be an option for Oslo CTM3, but this method is rather similar to the current approach.

8.8.6 Vertical distribution

Many CTMs distribute L-NOx vertically by using the vertical profiles of Pickering et al. (1998). Those profiles have recently been revised by Ott et al. (2010), where the “C-shaped” emission profile is replaced by a “backward-C” shaped profile, and is now the default distribution in the Oslo CTM3.

The vertical distribution (Ott et al., 2010) needs different geographic regions to be defined, and these are taken from Allen et al. (2010). The vertical profiles are scaled to match the height of the convective plumes, as found in the meteorological data.

When the Oslo CTM3 was in its early start, UCI CTM used a different vertical distribution, namely by Stockwell et al. (1999). This treatment placed lightning emissions too low in the atmosphere, and should not be used.

8.8.7 Lightning scaling factors

To match the lightning frequency in Eq. (96) to observed values, we need to find s_O and s_L (Eq. (100–99)). To find proper values, at least a whole year of meteorological data should be applied. Preferably, several years should be used, to create a climatological mean.

This calculation is already done in the lightning subroutine *lightning.f90*. Accumulated flash rates for land and ocean are calculated using the original Price and Rind (1992) equations scaled to grid box averages, i.e. Eq. (96), and from these the scaling factors are calculated. Running average values are printed to screen at the last meteorological time step of each day, average scaling factors are printed to screen. When you start a simulation at day 1, the annual average scaling factor is thus found at day 365.

The quickest way to generate scaling factors is to set `LIT=:Y` in *Makefile*, and use a stripped *pmain.f90* which only reads meteorological data and calculates lightning.

When you have a new meteorological dataset, you should let the model run through these calculations, and use the new factors to replace `scaleLand` and `scaleOcean`.

If you have one year of e.g. T159L60 and T42L60, and know the scaling factors for one of them, you may probably obtain suitable scaling factors without using the climatological values mentioned above, but instead calculate for one year of both datasets.

Alternative method

To make more specific calculations on the rates, e.g. standard deviations, you can also specify `getFlashFiles=.true.` in *lightning.f90*, to produce files containing the 3-hourly flash rates for both land and ocean. These files can be read using the IDL program *lightning_flashrate.pro* or the fortran program *lightning_flashrate.f90*, found in the repository utilities.

These files get rather big, and the IDL program may be very slow for high resolutions.

8.9 CH₄ emissions

Traditionally, CTMs have used fixed surface fields of CH₄, because of its relatively long lifetime in the atmosphere. It is now possible to rather run the Oslo CTM3 with emissions of CH₄. Whereas several emission datasets include anthropogenic CH₄ emissions (e.g. EDGARv4.2 and ECLIPSE), natural emissions are often not available. There is also soil uptake to be accounted for, a process that is not well quantified. Our current natural CH₄ source is generated by Bousquet for the GAME project, providing emissions from biomass burning, wetlands and oceans, and uptake by soil. This dataset also contain anthropogenic sources, which is not used in the Oslo CTM3.

What to remember when using CH₄ emissions (also described in the README file in model directory):

- `LOLD_TREATMENT=.false.` in *strat_h2o.f90*.
- Transport stratospheric H₂O, H₂ and H₂O_s; this requires `NPARTSTRAT` to be increased by 3 and `NOTRPARSTRAT` to be decreased by 2 in *cmn_size.F90*. This means that in the *tracer_list.d* file you have to move H₂ and H₂O_s to the transported section. And you have to add tracer number 114 H₂O.
- Increase JPPJ in *cmn_size.F90*, and add H₂O in *ratj_oc.d*. The entry is listed at the bottom of the file.
- Add H₂O in *FJX_spec.dat*; entry at the bottom of the file. You must also increase the first number on the second line of the file by 1; if this is 62, you change it to 63.
- Scale the CH₄ emissions up or down to match steady state. Or run the model until steady state is reached.
- Include appropriate CH₄ emissions in the emission file.
- If CH₄ dataset includes agricultural emissions, you need to turn off GFED emissions from that sector. This is done by the `partitions` variable in *emisutls_oslo.f90*.

Stratospheric H₂O

When calculating CH₄ emissions, stratospheric H₂O

must also be calculated. The old treatment, using the sum of H₂, 2xCH₄ and a fixed sum of these two and H₂O, will not hold when CH₄ is allowed to increase or decrease. That would require the sum of the three species is allowed to vary (on short time scales, at least).

So when CH₄ emissions are included, we also calculate gaseous H₂O in the stratosphere. It has a tropospheric source, due to upward transport, which is parameterized assuming tropopause H₂O to be 3.7 ppm, but limited to the saturation value (which is controlled by temperature).

Emission files

Anthropogenic emissions of CH₄ are available from several datasets, e.g. EDGAR v4.2 and CEDS. See *tables/EMISSION_LISTS* for options.

Natural CH₄ emissions are taken from Bousquet data, given in a file called *fch4.ref.mask11.nc*. Its natural sources are the fields biomass burning (`bbur`), wetlands (`wetlands`) and other sources (`other`). The Oslo CTM3 also reads the field `soils` in the deposition routine, to calculate surface dry deposition (see Section 7.2.5). Note that when biomass burning is included from the Bousquet data, the GFED data should not be used.

Important note

The CH₄ emissions must probably be scaled up or down to match the total loss in the model. If you are not familiar with this approach, ask the experienced users. Total CH₄ loss is written to standard out every month, and the emitted CH₄ should match this when in steady state.

8.10 Emission diagnoses

The emissions of each species are accumulated in the array `DIAGEMIS_IJ`. From this array, the daily accumulated global totals are found in the subroutine `tnd_emis_daily` in *diagnostics_general.f90*. At the dates specified by the diagnostics/budget calendar in *LxxCTM.inp* file, the following are done (subroutine `tnd_emis2file`):

- Globally accumulated emissions of each species since last printout are written to standard output (i.e. result file).
- The horizontal distribution of the accumulated emissions are written to files *emis_maps_YYYYMMDD.dta*. If emissions are located at several model levels, they are all written to file.
- Daily accumulated emission totals are written to file *emis_daily_totals_YYYY.dta*. These are only written at the days specified by the budget calendar.

If emissions are treated as a separate process, most of this diagnostic is unnecessary. However, since we treat emissions as production terms in chemistry, this diagnose must be included to assess what is actually emitted.

8.11 Pre-defined datasets

Here you can find some info on the different pre-defined collections of emission files. Generally, these can be found through the ECCAD (Emissions of atmospheric Compounds & Compilation of Ancillary Data)

web page <http://eccad.sedoo.fr/>. Emission lists can be found in the directory *tables* and the subdirectory *EMISSION_LISTS*. These latter lists have to be combined into a total emission list in *tables*. Some lists of both anthropogenic and natural emissions are already generated; see the *tables/Ltracer_emis.inp*-files.

Keep in mind which year the files are defined for! This is usually given by their file names.

8.11.1 CEDS

Lists for CEDS anthropogenic emissions can be found at *Ltracer_emis_ceds.dat*.

These are the CMIP6 emission datasets, but note that I have generated new files for the anthropogenic emissions. This is because the CEDS format is ill suited for extracting separate sectors.

CEDS has monthly variation.

8.11.2 ECLIPSE

Lists for ECLIPSE anthropogenic emissions can be found at *Ltracer_emis_eclipse5.dat* and *Ltracer_emis_eclipse4.dat*.

ECLIPSE includes the agricultural waste burning, which is usually a part of biomass burning. This means that when including GFED biomass burning, you have to skip that partition. This is hard-coded in the GFED routine, through the variable `partitions`,

ECLIPSE has no monthly variation; it is annual mean only.

8.11.3 EDGAR v4.2

EDGAR v4.2 anthropogenic emissions are available, and can be found in *Ltracer_emis_edgar42.dat*. This file contains CH₄ emissions, so if you use fixed surface CH₄, you cannot include those entries.

EDGARv4.2 has no monthly variation; it is annual mean.

8.11.4 Lamarque/IPCC

Lamarque et al. (2010) anthropogenic emissions *Ltracer_emis_lamarque.dat*.

The Lamarque dataset has a monthly variation.

8.11.5 HTAP

More information can be found at the HTAP web page <http://htap.org/>. HTAP emissions are given on a monthly time scale, and are based on EDGAR data. *Ltracer_emis_htap.dat*.

8.11.6 RETRO

RETRO anthropogenic emissions, combined with POET natural emissions (Granier et al., 2005; Olivier et al., 2003), can be found in *Ltracer_emis_retro.dat* in *tables/EMISSION_LISTS/*.

This dataset has a monthly variation.

8.11.7 POET

POET provided datasets of natural emissions from ocean. *tables/EMISSION_LISTS/Ltracer_emis_ocean.dat*.

8.11.8 CH₄ emissions Bousquet

Through the project GAME, a dataset of CH₄ emissions, based on Bousquet et al. (2011) was generated: *Ltracer_emis_ch4_bousquet.dat*.

Keep in mind that this dataset also includes biomass burning, so you must make sure CH₄ is not included in GFED.

The dataset contains several sources of CH₄, however, we have never used the anthropogenic part. Also soil sink is given.

Dataset has monthly variation for year 1984 – 2009.

8.11.9 Volcanic emissions

Volcanic emissions of SO₂ was provided by both AEROCOM and later HTAP: *Ltracer_emis_volcanoes.dat*.

Note that HTAP emissions are based on volcanic events, so make sure the emissions actually cover your simulation period.

8.11.10 Soil emissions

Soil emissions for some species: *Ltracer_emis_soils.dat*.

8.11.11 Biomass burning

Lists for biomass burning (CEDS and GFEDv4) emissions can be found at *Ltracer_emis_biomassburning.dat*.

9 QSSA chemical integrator

The numerical integration of chemical kinetics is done applying the Quasi Steady State Approximation (QSSA) introduced by Hesstvedt et al. (1978), using three different integration methods depending on the chemical lifetime of the species, to save computing time.

For a given integration time step Δt , the definition of the three methods are

- Longlived: $\text{Loss} < 0.1/\Delta t$

- Shortlived: $\text{Loss} > 10/\Delta t$
- Intermediate: $0.1/\Delta t \leq \text{Loss} \leq 10/\Delta t$

The change of a tracer concentration depends on the production and loss terms

$$\frac{dC}{dt} = P - LC \quad (108)$$

where C is tracer concentration [molec/cm³], P is production [molec/(cm³s)] and L is loss rate [1/s].

Re-arranging, we get

$$\frac{dC}{P - LC} = dt \quad (109)$$

which can be integrated using the kernel rule:

$$-\frac{1}{L} d\ln(P - LC) = dt \quad (110)$$

Integrating from (C_1, t_1) to (C_2, t_2) , we have

$$\frac{P - LC_2}{P - LC_1} = e^{-(t_2 - t_1)L} \quad (111)$$

Setting $\Delta t = t_2 - t_1$ and solving for C_2 we get

$$C_2 = \frac{P}{L} + (C_1 - \frac{P}{L})e^{-L\Delta t} \quad (112)$$

9.1 Longlived species

Longlived species have small L and we can approximate

$$\exp(-L\Delta t) \approx 1 - L\Delta t \quad (113)$$

and using this, Equation (112) becomes

$$C_2 = C_1 + (\frac{P}{L} - C_1)L\Delta t \quad (114)$$

9.2 Shortlived species

Shortlived species have larger L and we can approximate

$$\exp(-L\Delta t) \approx 0 \quad (115)$$

and get

$$C_2 = \frac{P}{L} \quad (116)$$

However, for $P = 0$, shortlived species are treated like intermediate species.

9.3 Species of intermediate lifetime

Species of intermediate lifetime and shortlived species without production terms are integrated using the full Equation (112).

10 Tropospheric chemistry

The tropospheric chemistry routine is in principle a 1D model, looping through a column. It is turned on by setting `TROP_CHEM :=Y` in the user specified section of *Makefile*.

The tropospheric chemistry was first introduced in the CTM-1 (Berntsen and Isaksen, 1997), and in its general form it contains 46 components given in Table 15. Originally there were 51 species, but 2 were not used (nr 26: CH₂O₂OH and nr 47: DMS, which has a new number in sulphur scheme) and are removed in the Oslo CTM3. Also the NOX and NOZ families used to be unnecessarily transported, so they have been put solely into the chemistry. O₃NO (O₃-NO) is also treated in chemistry only (commented in Section 2.5).

Transporting a species with lifetime much shorter the transport time step (usually 15 minutes for boundary layer mixing/chemistry) may seem inconsistent, because the species may have changed a lot during transport. Therefore, some tracers have not been transported in Oslo CTM3, listed with a **No** in the Table 15. See Section 10.1 for more on this.

Some species in Table 15 are labeled **Maybe**, indicating that they may be left out of transport. I advise against this. Species should either be transported or set from some steady state initial value in the chemistry routines.

Tropospheric water vapor is set from meteorological data and is kept fixed for the whole meteorological time step.

10.1 Non-transported species

One issue that has to be resolved in the Oslo CTM3 is that non-transported species should not be used as historic values: After other species have been transported, the non-transported species should not be used in chemistry for the same grid box. Instead some initial steady state value should be calculated before chemistry. Then the array of non-transported species could be removed or kept as a diagnostic tool.

Be sure that if the species labeled **Maybe** in Table 15 are removed from transport, you should set initial values in the chemistry. These will have to be hard coded to some steady state expression/value, and should *never* be from a non-transported array.

It can be argued that transporting very shortlived species (labeled **No** in Table 15) makes little sense, since the tracer concentration will have changed before getting to a new location. However, we still keep some tracers in the non-transported array. I mention again that historical values of the non-transported tracers are of little value, and in worst case erratic. For OH this may not be a big problem, due to the iteration to get a stable value, although the old value is used for some calculations before the new value is calculated.

Table 15: The components of the tropospheric chemistry application. The table gives order of magnitude estimates of the lifetime of the components. If the lifetime is short, there is no need for transport.

| Nr | Component name | Remarks | Approximate lifetime | Transport | Wet dep. |
|----|---|---|----------------------|-----------|----------|
| 1 | O ₃ | Ozone | ~ months | Yes | Yes |
| 4 | HNO ₃ | Nitric acid | ~ weeks | Yes | Yes |
| 5 | PANX | PAN + CH ₃ COO ₂ | | Yes | No |
| 6 | CO | | | Yes | No |
| 7 | C ₂ H ₄ | Ethene [CH ₂ CH ₂] | | Yes | No |
| 8 | C ₂ H ₆ | Ethane [CH ₃ CH ₃] | | Yes | No |
| 9 | C ₃ H ₆ | Propene [CH ₃ CHCH ₂] | | Yes | No |
| 10 | C ₄ H ₁₀ | Butane [CH ₃ CH ₂ CH ₂ CH ₃] | | Yes | No |
| 11 | C ₆ H ₁₄ | Dimethylbutane | | Yes | No |
| 12 | C ₆ HXR | m-Xylene/1,3-Dimethylbenzene [C ₈ H ₁₀] | | Yes | No |
| 13 | CH ₂ O | Formaldehyde | | Yes | Yes |
| 14 | CH ₃ CHO | acetaldehyde | | Yes | Yes |
| 15 | H ₂ O ₂ | hydrogenperoxide | | Yes | Yes |
| 16 | CH ₃ O ₂ H | methyl hydroperoxide | | Yes | Yes |
| 17 | HO ₂ NO ₂ | Peroxynitric acid | | Yes | Yes |
| 18 | CH ₃ COY | Bi-acetyl [CH ₃ COCOCH ₃] | | Yes | No |
| 19 | C ₃ COX | Methylethyl ketone (2-butanone), CH ₃ COC ₂ H ₅ | | Yes | No |
| 20 | ISORPRENE | Isoprene/2-methylbuta-1,3-diene [C ₅ H ₈] | | Yes | No |
| 21 | HO ₂ | | short | Maybe | No |
| 22 | CH ₃ O ₂ | methyldioxy radical | short | No | No |
| 23 | C ₂ H ₅ O ₂ | ethyldioxy radical | short | No | No |
| 24 | C ₄ H ₉ O ₂ | butyldioxy radical | short | No | No |
| 25 | C ₆ H ₁₃ O ₂ | | short | No | No |
| 27 | CH ₃ COB | RO ₂ from C ₄ H ₁₀ +OH, CH ₃ COCH(O ₂)CH ₃ | | Yes | No |
| 28 | CH ₃ CXX | CH ₃ CH(O ₂)CH ₂ OH | | Yes | No |
| 29 | AR1 | RO ₂ from C ₆ HXR + OH | short | Maybe | No |
| 30 | AR2 | Ketone from AR1 | | Yes | No |
| 31 | AR3 | RO ₂ from AR3 | short | Maybe | No |
| 32 | ISOR1 | RO ₂ from ISOPRENE + OH | short | Maybe | No |
| 33 | ISOK | methylvinylketone + methacrolein (ketones) | | Yes | Yes |
| 34 | ISOR3 | RO ₂ from ISOK | short | Maybe | No |
| 35 | HCOHCO | Glyoxal | | Yes | No |
| 36 | RCOHCO | Methyl glyoxal, CH ₃ COCHO | | Yes | No |
| 37 | CH ₃ X | Peroxyacetyl radical, CH ₃ COO ₂ | | Yes | No |
| 38 | O(³ P) | | short | No | No |
| 39 | O(¹ D) | | short | No | No |
| 40 | OH | | short | No | No |
| 41 | NO ₃ | | | Yes | No |
| 42 | N ₂ O ₅ | | | Yes | No |
| 43 | NO | | | Yes | No |
| 44 | NO ₂ | | | Yes | No |
| 46 | CH ₄ | Methane | ~ years | Yes | No |
| 48 | C ₃ H ₈ | Propane | | Yes | No |
| 49 | C ₃ H ₇ O ₂ | Propyl peroxide; from (propane+OH)+O ₂ | | Yes | No |
| 50 | Acetone | CH ₃ COCH ₃ | | Yes | No |
| 51 | C ₃ COD | Propyldioxy, 2-oxo-propyldioxy, CH ₃ COCH ₂ (O ₂) | | Yes | No |

10.2 Tropospheric domain

When running tropospheric chemistry, you may or may not include stratospheric chemistry (see Section 11 for stratospheric chemistry).

If you run *without* stratospheric chemistry, tropospheric chemistry is calculated up to a certain altitude, but when running full chemistry (stratospheric chemistry included) it stops at the actual tropopause level for each column.

The tropopause level for a grid box is defined by the global array `LMTROP` (see Section 20.1).

It is also possible to use the `e90`-tracer to define stratospheric air (Section 21.1.3), either as a 3D field or by selecting the uppermost tropospheric grid box as tropopause. The program code is not set up for a 3D definition.

10.3 Without stratospheric chemistry; O₃, NO_x and HNO₃

O₃, NO_x and HNO₃ are very important in the stratosphere, and are transported down into the troposphere. In Oslo CTM2 a flux of O₃ was set in the uppermost model layer (the SynOz approach, McLinden et al. (2000)), but this is only possible for L40 vertical resolution. We have left this behind, and now use a climatology calculated from a full-chemistry T42L60 simulation for the years 2000–2008.

For each model latitude band (for each J), tropospheric chemistry is calculated up to a few levels above `max(LMTROP(:,J))`. The number of levels added are controlled by the parameter `LVS2ADD2TC` in `cmn_oslo.f90`. Above this, O₃ is set from the model climatology.

The climatology of O₃ also affects `D03` used in calculation of photochemical reaction rates (Section 12).

Above `max(LMTROP(:,J))+LVS2ADD2TC` we also set HNO₃ and NO_x species based on climatologies. For consistency, these are from the same T42L60 simulation as the O₃ climatology. This is carried out to improve important UTLS NO_x chemistry.

The old Oslo CTM2 method is still available, but should not be used. It was based on observed mixing ratio (μ) correlations of NO_y with O₃, assuming 40% to be NO_x=NO and 60% to be HNO₃:

$$\begin{aligned}\mu_{HNO_3} &= 0.0024\mu_{O_3} \\ \mu_{NO} &= 0.0016\mu_{O_3}\end{aligned}$$

The routines are shortly described in Appendix A.2.41.

10.4 Box version of tropospheric chemistry code

A box version of the tropospheric chemistry code was produced by Alf Grini and it is available in the Oslo CTM3 tool box at `/div/amoc/d4-4/oslo-ctm/archive_ctm/box_models/`.

This directory includes some matlab scripts which will plot the concentration daily cycles. The box can be a good educational tool, and has been used in a bachelor level atmospheric chemistry course.

A user manual for the box application is available as text file in the `photochem_box/manual`-directory.

11 Stratospheric chemistry

The stratospheric application is turned on by setting `STRATCHEM :=Y` in the user specified section of *Makefile*.

Species treated in the stratospheric chemistry are listed in Table 16. As for tropospheric chemistry there are some non-transported species, which should either be changed into transported species or set inside chemistry. E.g. H₂ must be transported when stratospheric H₂O is calcu-

lated (Section 11.2), but should otherwise be a static field.

The stratospheric chemistry was originally based on the Oslo 2D model (Stordal et al., 1985), later included in the stratospheric 3D model Oslo SCTM-1 (Rummukainen, 1996; Rummukainen et al., 1999) before included in the Oslo CTM2 (Gauss, 2003; Søvde et al., 2008).

Table 16: The components of the stratospheric application. Trsp. denotes transport or not.

| Nr | Component | Remarks | Trsp. |
|-----|--------------------------------|--|--------|
| 101 | MCF | CH ₃ CCl ₃ | Yes |
| 102 | HCFC22 | CHF ₂ Cl | Yes |
| 103 | CFC11 | CCl ₃ F | Yes |
| 104 | CFC12 | CCl ₂ F ₂ | Yes |
| 105 | CCl ₄ | | Yes |
| 106 | CH ₃ Cl | | Yes |
| 107 | N ₂ O | | Yes |
| 108 | Clx | | Yes |
| 109 | NO _x _str | | Yes |
| 110 | SO | O ₃ + O(³ P) + O(¹ D) - NO - Cl - Br | Yes |
| 111 | HCl | | Yes |
| 112 | Cl _y | | Yes |
| 113 | H ₂ | | No/Yes |
| 114 | H ₂ O | May be used | |
| 115 | SH | H + OH + H ₂ O ₂ | Yes |
| 116 | CH ₃ Br | | Yes |
| 117 | H1211 | CF ₂ ClBr | Yes |
| 118 | H1301 | CF ₃ Br | Yes |
| 119 | Bry | | Yes |
| 120 | H2402 | CF ₂ BrCF ₂ Br | No |
| 121 | F113 | CF ₂ ClCFCl ₂ | Yes |
| 122 | F114 | CF ₂ ClCF ₂ Cl | Yes |
| 123 | F115 | CF ₃ CF ₂ Cl | Yes |
| 124 | HNO ₃ s | Solid HNO ₃ | Yes |
| 125 | H ₂ Os | Solid H ₂ O | Yes |
| 126 | HCl _s | Not in use | |
| 127 | HCFC123 | CF ₃ CHCl ₂ | Yes |
| 128 | HCFC141 | CF ₃ FCI ₂ | Yes |
| 129 | HCFC142 | CF ₃ CF ₂ Cl | Yes |
| 130 | H | | No |
| 131 | HNO ₂ | Not in use | |
| 132 | Cl | | No |
| 133 | ClO | | Yes |
| 134 | OHCl | | Yes |
| 135 | ClONO ₂ | | Yes |
| 136 | Cl ₂ | | Yes |
| 137 | OCIO | | Yes |
| 138 | HBr | | Yes |
| 139 | Br | | Yes |
| 140 | BrO | | Yes |
| 141 | BrONO ₂ | | Yes |
| 142 | OHBr | | Yes |
| 143 | Br ₂ | | Yes |
| 144 | ClOO | | Yes |
| 145 | Cl ₂ O ₂ | | Yes |
| 146 | BrCl | | Yes |
| 147 | NO _y _str | | Yes |

11.1 Technical information

The stratospheric master routine is called from the chemistry master routine in *main_oslo.f90*. Working on an IJ-block (Section 4.3.2), it loops first through the latitudes and longitudes of the IJ-block, calling the chemistry (OSLO_CHEM_STR_IJ) column-wise.

Reaction rates dependent on temperature and pressure are defined as arrays of length LPAR, but only the stratospheric values are calculated, i.e. from LMTR0P+1 to LPAR (even though chemistry is not currently calculated in LPAR). Although the tropospheric part of the arrays are not used, this approach is faster than allocating the arrays on the fly. In addition, the arrays are small and minimal in numbers. Also heterogeneous reaction rates are calculated in this way.

11.2 Stratospheric H₂O

In general H₂O is not transported in the Oslo CTM3; tropospheric H₂O is set from the meteorological data, while stratospheric H₂O is calculated from the sum of potential hydrogen, denoted sumH2, as:

$$\text{H}_2\text{O} = \text{sumH}_2 - 2\text{CH}_4 - \text{H}_2 \quad (117)$$

where sumH₂ = 7.72 ppmv (Zöger et al., 1999). The old sum was 6.97 ppmv, which was slightly low, although the difference did not change the chemistry much.

Note that this value has to be lowered if you simulate pre-industrial times..

It is also possible to transport H₂O and calculate H₂O in the stratospheric chemistry, by setting `L0LD_H20TREATMENT=.false.` in *strat_h2o.f90*. If you want to do this, you need to

- Set `L0LD_H20TREATMENT=.false.`
- Transport H₂O (component 114), H₂ (113) and solid H₂O (125), i.e. in *cmn_size.F90* you must add 3 (113, 114 and 125) to `NPAR_STRAT` and remove 2 from `NOTRPAR_STRAT` (113 and 125).
- Include cross section information for fast-JX in *FJX_spec.dat*, put them after Acet-b (H₂O values can be found in *FJX_spec_h2o.dat*).
- Add 1 to the first two numbers in the header of *FJX_spec.dat*, i.e. change 62 to 63.
- Also add H₂O in *ratj_oc.d*.
- In *cmn_size.F90* you must add 1 to `JPPJ`.

Tropospheric source of stratospheric H₂O

H₂O is transported throughout the model domain. However, we only calculate H₂O chemistry in the stratosphere. In the troposphere, H₂O is set from the meteorological data. Consequently, our H₂O tracer is a purely stratospheric tracer, with a tropospheric source. The tropospheric source is set before transport, and is calculated assuming a mixing ratio of 3.7 ppm at the tropopause, but limited to saturation mixing ratios.

To avoid large values coming up, the tropospheric values are set in the tropopause level and 4 levels below it. From there and down to the surface, a very small value is set.

In this treatment, H₂O mixing ratio in the uppermost model layer is assumed to be the same as in the layer below (routine `strat_h2o_ubc2` in *strat_h2o.f90*).

Important

This new H₂O treatment is better than the old version, which should eventually be abandoned. It should be applicable also for pre-industrial simulations, assuming the tropopause mixing ratio has not changed much. However, tropopause temperatures may indeed have changed, but the largest contribution to changes in stratospheric H₂O from pre-industrial times is due to increased CH₄.

Further testing is needed before using the new treatment widely.

11.3 Microphysics

The microphysics scheme calculates the formation and evolution of polar stratospheric clouds (PSCs). It is a column model, which fits very well into the IJ-block structure. The microphysics are explained in detail by Søvde et al. (2008), but will be included here as well.

You can turn off PSC heterogeneous chemistry by the logical `LPSC` in *psc_microphysics.f90*, where you also can turn off heterogeneous chemistry on stratospheric background aerosols (`LAEROSOL`).

The calculated surface area densities `PSC1` and `PSC2` are given in global fields of size (LPAR,IPAR,JPAR). These are used to calculate reaction rates in the stratospheric chemistry master routine.

An important aspect of this microphysics is that sulfuric acid (H₂SO₄) is needed in the calculations. As long as H₂SO₄ is not calculated as a species in the stratosphere, it is computed from an existing background aerosol distribution (see Section 11.4), assuming some content of H₂SO₄ (see Søvde et al. (2008) for more). As explained in the following text, the background aerosol surface area may be modified by the microphysics scheme, and to keep the consistency, the amount of sulfuric acid is always computed from the original satellite data.

Important

The PSC microphysics module limits calculations to an altitude of 28 km. This is to reduce the number of unnecessary calculations. However, it means that for other aerosols, the satellite based surface aerosol density will be used. It could be that using the PSC microphysics above 28 km could alter possible aerosols there.

Formation

Given an amount of HNO₃, H₂SO₄ and H₂O, the composition of a ternary solution is calculated according to Carslaw et al. (1995). This includes HNO₃ freezing on ice assuming 3 K supercooling below *T_{ICE}* from Marti and Mauersberger (1993):

$$T_{ICE} = \frac{2663.5}{12.537 - \log_{10} p_{H_2O}} \quad (118)$$

with *p_{H₂O}* in Pa.

The formed particle is treated as background aerosols (temporarily overwriting the background aerosol satellite data) unless the temperature is below *T_{NAT}* given by

Hanson and Mauersberger (1988) for pressures in Torr:

$$\begin{aligned}\log p_{\text{HNO}_3} &= m(T) \log p_{\text{H}_2\text{O}} + b(T) \\ m(T) &= -2.7836 - 0.00088T \\ b(T) &= 38.9855 - \frac{11397}{T} + 0.009179T\end{aligned}\quad (119)$$

At equilibrium we have $T = T_{\text{NAT}}$. Below this temperature the particle is treated as supercooled ternary solution (STS, also known as PSC1b).

Further, this ternary solution is assumed to be liquid until freezing at a temperature

$$T_{\text{FRZ}} = \frac{-9384}{\log_{10}(p_{\text{HNO}_3} p_{\text{H}_2\text{O}}) - 39} \quad (120)$$

where the pressures are in Torr. This expression is close to the freezing temperature SAT:MixH reported by Fox et al. (1995), of a mixture of SAT ($\text{H}_2\text{SO}_4 \cdot 4\text{H}_2\text{O}$) and $\text{HNO}_3 \cdot \text{H}_2\text{SO}_4 \cdot 5\text{H}_2\text{O}$. T_{FRZ} is in general 3-6K lower than T_{NAT} , in agreement with several studies (e.g. Voigt et al., 2005).

The particle is then assumed to be nitric acid trihydrate (NAT, or PSC1a). Once formed, the NAT will stay NAT until it melts at the temperature reported by Zhang et al. (1993):

$$T_{\text{MELT}} = \frac{3236}{11.502 - \log_{10} p_{\text{H}_2\text{O}}} \quad (121)$$

where $p_{\text{H}_2\text{O}}$ is in Torr.

Søvde et al. (2011b) let the NAT particles grow, also letting the volume of PSCs grow without a limit, whereas the original treatment in Søvde et al. (2008) used a volume limit as in the routine it was based on. We keep this limit in Oslo CTM3 because otherwise the particle area density will grow too large. This was never an issue in the Antarctic, but made too large PSCs when modelling the 2011 Arctic spring.

Sedimentation

Sedimentation is done according to Kasten (1968) for each size bin in the log-normal size distributions.

11.4 Heterogeneous chemistry

In Oslo CTM3 stratosphere, heterogeneous chemistry comprises reactions on PSCs and background aerosols. The reaction rates depend on the surface area density of the particles, which are either given by monthly averaged satellite data or calculated by the microphysics scheme (see Section 11.3).

11.5 Input files needed

The stratospheric module needs information about stratospheric background aerosols and also boundary conditions for the species treated only in the stratosphere (surface conditions to simulate emissions, and upper boundary conditions to simulate interaction with the atmosphere above).

The data are located in the directory *Input_CTM3*:

- Climatological background aerosol data are given in the directory *backaer_monthly* (described in Section 2.7.8).

- Boundary conditions generated from the Oslo 2D model are located in the directory *2d_data*. Note that the last year of data is for 2011 due to the Oslo 2D model being discontinued. See also next Section for upper boundary alternatives.

You also need to have the correct tracer list *tracer_list.d*, with the correct number of species, which you can find in the directory *tables/*.

11.6 Upper boundary / Chemistry in LPAR?

So far, the Oslo CTM3 and Oslo CTM2 have not calculated chemistry at the top model layer (LPAR). This may be revised in the future.

The use of Oslo 2D data as upper boundary conditions must be revised! The uppermost level of the 2D model is about 55km, well below the L60 top level. Using 2d-data is ok for L40, but not ideal for L60. However, in lack of other boundary conditions we scale the 2D data to L60 using the uppermost mixing ratio gradient.

The best solution is to do chemistry for all species in LPAR. However, it can be tricky for some tracers if a flux in or out is needed, such as species with long stratospheric lifetimes where the mesosphere provides an important sink. Although a bit tricky, that should rather be parameterised.

Using another model (e.g. WACCM) or observations as upper boundary condition is better than using Oslo 2D results. However, any fixed upper boundary will possibly act as a sink or source, and the upper boundary will depend on whether pre-industrial, current or future atmosphere is modelled.

If chemistry is to be calculated in LPAR, this must be done:

- Reaction rates dependent on temperature and pressure must be calculated in LPAR (in subroutine *TCRATE_TP_IJ_STR* and *TCRATE_HET_IJ*).
- The routine updating the upper boundary must be removed (*update_strat_boundaries* in *stratchem_oslo.f90*).
- Climatological O_3 , temperature and mass for layer LPAR, used in *photoj* must be removed. Can also be removed from *set_atm* in *fastjx.f90*.

11.7 Linoz

Linoz v2 (McLinden et al., 2000) is included in the file *p-linoz.f*. However, the Oslo CTM3 is not set up to use this instead of stratospheric chemistry, only as part of the STE diagnostic tool (Section 21.1.4).

However, all UCI Linoz codes are present, so setting it up as an alternative stratosphere should be rather straightforward.

12 Photochemistry

The photodissociation rates (J-values) are calculated online using the fast-JX method, version 6.7c (Prather, 2012). fast-JX calculates dissociation rates in the troposphere and stratosphere. When treating only the troposphere, there are 20 values calculated, and for the stratospheric application there are 49. The parameter name for this is JPPJ and is automatically set in *cmn_size.F90*. The reactions are listed in *ratj_oc.d*.

You can set up the model to calculate J-values every chemical time step (NRCHEM), or to calculate only once every step of the operator split (NOPS). This is controlled in the input file (see Section 2.7.3) using the parameter LJCCYC (J-values constant in the chemistry cycle). Each parallel block (IJ-block) calculates its J-values, and stores them in the array JVAL_IJ, which is a global B-like array of size (JPPJ, LPAR, IDBLK, JDBLK, MPBLK). This minimizes the striding necessary for each parallel block.

The master routine is *jvalues_oslo*, where J-values for each column is calculated by the driver *jv_column*, and stored in the global JVAL_IJ. These subroutines are located in *main_oslo.f90* (see Appendix A.1.37 and A.2.26).

The driver calls the fast-JX routine PHOTOJ located in the file *p-phot_oc.f*.

The fast-JX uses the ozone column to calculate radiative properties. To account for the atmosphere above the model, a climatology is applied. This is carried out in the subroutine SET_ATM in *fastjx.f90*.

SET_ATM provides information about what is above the model top (above ETAA(LPAR+1)) as

- TOPT: Temperature
- TOPM: Mass
- TOP3: O3 concentration

In addition we have computed the values for layer LPAR (between ETAA(LPAR) and ETAA(LPAR+1)), since a climatology is thought to be more reliable than the 2D upper boundary conditions. These arrays are LPART, LPARM and LPAR3.

Important input to the J-values are cloud cover and aerosol distribution, since they have important scattering properties, and these will be addressed next. First a short note about solar flux.

12.1 Solar flux

The solar flux is listed at the top of the table *FJX_spec.dat*, named SOL#/cm²/s. It is the average of solar low (11 Nov 1994) and 80% of solar high (29 Mar 1992). The values apply for the wave lengths given in the same file. The values are from the Solar-Spectral Irradiance Monitor (SUSIM).

The solar low and solar max values are found in the file *FJX_solminmax.dat*. It is possible to include an interpolation between these based on observed solar cycle. See *fastjx.f90* and search for FLmin or FLmax to find out more. I am not completely sure that a linear interpolation be-

tween min and max is correct for all wave length bins, but it is the easiest way to do this at the moment.

Solar flux can be found at Natural Resources Canada, <http://www.spaceweather.gc.ca/solarflux/sx-5-en.php>, and when I tested this I made 7-month running mean of the fraction of maximum flux (i.e. 1 is max and 0 is solar min). A file can be found in the *tables* directory: *solflux_7month_running_mean_1990_2016.dat*. You have to specify FLscale (see *fastjx.f90*) fits the number of years in this file.

Note that including the solar cycle will only affect photochemistry. This effect is not so large as the effect of changed atmospheric temperatures, which is already included in the meteorological data.

12.2 Cloud cover

If no clouds are found in a model column, the J-values in a model column are calculated straight-forward; only one calculation is necessary. Clouds, however, makes the calculations more complicated.

In a given model column, there may be different types of clouds with different cloud fractions, which may overlap or not. Using the cloud cover in the meteorological data, there are several ways to calculate the cloud optical properties used for J-values in fast-JX.

How to treat the clouds in fast-JX is defined in the *LxxCTM.inp*-files, where you can set a random cloud cover treatment; so if you set all to false, the result will be the classic average cloud cover as in Oslo CTM2. The default treatment is LCLDRANA.

The treatment of overlapping clouds is described by Neu et al. (2007), and is also described shortly below.

12.2.1 Average cloud cover

Average cloud cover means that clouds covering a fraction of a gridbox is averaged to a cloud covering the whole grid box. E.g. a convective cloud with optical depth of 20 covering 20% of the grid box, will be treated as a cloud covering the whole grid box by an optical depth of 4. Neu et al. (2007) showed that this is not a good approximation.

12.2.2 Random cloud cover

Clouds with cloud fraction (CF) less than 1 does not cover the whole grid box. They may be located at different places and they may overlap. There are two main types of treating this overlap; random and maximum-random overlap (Neu et al., 2007).

In the Oslo CTM3 the calculations are carried out over NDGRD=IDGRD×JDGRD columns of cloud properties. IDGRD=IPARW/IPAR, and similarly for JDGRD; in other words they will be 1 for non-degraded horizontal resolution. NDGRD is therefore the number of native columns covered by a column in a degraded run. For non-degraded, NDGRD=1. For a degraded-grid simulation

where each column covers several native columns, the native information from the meteorological data is used.

For each column the clouds are grouped into maximum-overlapping clouds: Clouds from neighboring levels are expected to be closely connected and assumed to form a maximum-overlap group.

For each maximum-overlap group, the number of possible combinations of columns are calculated. These are the independent cloud atmospheres, ICAs). In this process, as described by Neu et al. (2007), the total number of ICAs has been reduced by grouping cloud fractions into bins (there are `CBIN_` of them (set in `cmn_fjx.f90`).

For each ICA the total column optical depth (TOD) is calculated. How the TOD values are treated depends on your random scheme choice. The TOD values are the basis for creating 4 quadrature atmospheres (QA), which are defined by optical depths:

- QA(1): 0-0.5 (clear sky)
- QA(2): 0.5-4 (cirrus hazy)
- QA(3): 4-30 (stratus)
- QA(4): >30 (cumulus)

For further reading see Neu et al. (2007). As a general user, your choices are to set the `LxxCTM.inp` switches, which are:

LCLDQMD

Use mid-point of quadrature cloud cover ICAs. This is the original method published by the UCI group (Neu et al., 2007). It generates all the possible max-ran overlap cloud profiles, then sorts them in order of increasing optical depth (OD), and breaks those into 4 groups based on the standard breakpoints defined above.

Next, each group (may be less than 4) has a fractional area, from which the mid-point of that area is picked to find the ICA that is used.

This is the most expensive because it sorts a large number of ICAs and then results on average in 2.5 to 2.8 calls to fast-JX per time step.

LCLDQMN

Mean quadrature cloud cover ICAs. Generates all max-ran ICAs and then averages them into the four quadrature bins. No sorting by OD, but still used up to 4 ICAs per step.

LCLDRANA

Random selected from all cloud cover ICAs. This is the cheapest and fastest - it picks a random number (fractional area = 0-1) and then generates the ICAs until it reaches that fractional area and selects that ICA. No sorting and only 1 call to fast-JX per time step. This is the default.

LCLDRANQ

Random selected from 4 mean quadrature cloud cover ICAs. Generates the ICAs and up to 4 quad atmospheres (as for LCLDQMN), but then picks one of the 4 based on a random number.

12.3 Aerosols in fast-JX

fast-JX can handle different aerosol types, usually fetched from the tracer array (STT), but can also be set from climatologies. The arrays and routines used for this is found in `aerosols2fastjx.f90`, where climatologies from previous simulations also can be read in.

You can turn off the effect of aerosols on fast-JX with the switch `LJV_AEROSOL` in `aerosols2fastjx.f90`. Here you also define which aerosols that can affect fast-JX. If you do a simulation without these aerosols, fast-JX will skip them also, unless a climatology is read in.

Aerosols may grow in size due to relative humidity (RH), and the optical properties for such aerosols are treated slightly different than for dry aerosols. The properties are listed in the files `tables/FJX_scat.dat` for aerosols independent of RH and `tables/FJX_UMaer.dat` for RH-dependent. These files will be further described in Section 12.5.

Using this module requires initialisation (separate routine in the module) and then to set the aerosol path arrays before fast-JX. This is done in `main_oslo.f90`.

Each aerosol type to include must be given a matching entry in the files listing optical properties (`tables/FJX_scat.dat` or `tables/FJX_UMaer.dat`). The scattering properties themselves are described in the respective aerosol sections.

If climatologies are used, they are given as monthly means of aerosol paths and are interpolated linearly in time, between two monthly means, at 00UTC every day.

If you change or add aerosol types, you may need to do changes in this module.

12.4 Generating cross sections

A program is available on Prather's web page, that allows you to generate cross sections. You only need to write your own small subroutine, which should be fairly easy after looking at the existing ones. You will need to look up JPL (Sander et al., 2006, 2011) or IUPAC (Atkinson et al., 2010) to get the data needed. You can also find a version of this program in the utilities repository (see Appendix B.1).

12.5 Generating scattering properties

When an aerosol is taken into account by fast-JX, its scattering and extinction properties are needed. You find pre-calculated values for aerosols independent on humidity in the file `FJX_scat.dat`, while scattering properties for aerosols depending on humidity can be found in `FJX_UMaer.dat`.

There are several ways to generate these numbers. The original one is by the program `FJ_phase`.

The better option is, however, a method by Mishchenko. It is better documented and also works better for producing humidity dependent parameters for `FJX_UMaer.dat`. See Section 12.5.2 for more.

Both methods can be found in the utilities repository (see Section B.1 to find where).

An entry in the *FJX_scat.dat* is shown in Table 17.

An aerosol entry in *FJX_UMaer.dat* consists of 21 lines covering optical parameters for relative humidity 0% to 95 % with increments of 5, and finally adding 99%. For 6 wavelengths, 200 nm, 300 nm, 400 nm, 550 nm, 600 nm and 1000 nm, 3 optical variables are stored: single scattering albedo, asymmetry parameter (g) and the extinction coefficient (Q_{ext}).

Size bins / Monodisperse particles

Some aerosols are assumed to have fixed size, as for dust and sea salt, so that several tracers make up the size distribution. Separate properties may then be calculated assuming monodisperse aerosols, as explained in the Mishchenko code.

12.5.1 FJ_phase

This is the generator I got from UCI, originating from Hansen and Travis (1974). The process is as follows:

- Compile *mie.for*.
- `mie < mie.in > mie.out`
- Compile *leg_mieout.for*.
- `leg_mieout < mie.out > leg.out`; `leg.out` contains the Legendre expansion, plus phase function vs. angle. The *FJX_scat.dat* values are found in the file `fort.7`.

You may also do the following:

- Compile *rd_mieout.for*.
- `rd_mieout < mie.out`; Look at `stdout` and check summary of aerosol distributions.

mie.in

The *mie.in* file consists of these parameters:

NSTEPS

The NSTEPS are set up to feed into the Legendre fitter that is the second part of the code, do not change these unless you want more forward peak resolution. It breaks the solution at the scattering phase angle into sections of different resolution (more at the forward and backward peak as noted).

NSD

Size distribution type. All are described in Hansen and Travis (1974).

- 1 Two-parameter Gamma function.
- 2 Bi-modal Gamma function.
- 3 Log-normal.
- 4 Power law.

IPART and NG

IPART and NG are for the integration over the size distribution (R). This is obscure, but historical in a way I haven't fully figured out. The size distribution is broken into IPART segments and each segment is then integrated over R in the range from `RBOT` to `RBOT + RDIV` using NG (96 in this case) Gauss-point quadrature. Thus

the NG*IPART is the effective number of R's used to integrate the scattering.

A, B, C

The parameters A, B and C depends on the size distribution.

NSD=1; Gamma function

$$n(r) = \text{constant } r^{(1/B-3)} \exp(-r/(AB)) \quad (122)$$

where the constant is given in the fortran program and

$$\begin{aligned} A &= \text{effective radius} \\ B &= \text{effective variance} \end{aligned}$$

This probably comes from Deirmendjian's modified GAMMA (pure GAMMA when $\gamma = 1$)

$$n(r) = ar^\alpha \exp(-br^\gamma) \quad (123)$$

$$N = a/\gamma b^{-(\alpha+1)/\gamma} \Gamma[(\alpha+1)/\gamma] \quad (124)$$

The mode radius is r_c :

$$r_c^\gamma = \alpha/(\gamma * b) \quad (125)$$

where

$$\begin{aligned} \alpha &= \text{dimensionless integer} \\ b &= \text{has units of } 1/\text{radius} \end{aligned}$$

Lacis's GAMMA: (NSD=1)

$$A = (\alpha + 3)/b = r_{eff} \quad (126)$$

$$\Rightarrow 1/b = r_{eff}/(\alpha + 3)$$

$$B = 1/(\alpha + 3) \quad (127)$$

$$r_c = A * B * (1/B - 3) = A * (1 - 3 * B) \quad (128)$$

$$r_c = r_{mode} = r_{eff} * \alpha/(\alpha + 3) \quad (129)$$

NSD=2; bi-modal Gamma distribution

$$\begin{aligned} n(r) &= \frac{1}{2} \frac{r^{1/B-3} \exp[-\frac{r}{AB}]}{(AB)^{(1/B-2)} \Gamma[1/B-2]} \\ &+ \frac{1}{2} \frac{r^{1/B-3} \exp[-\frac{r}{CB}]}{(CB)^{(1/B-2)} \Gamma[1/B-2]} \end{aligned} \quad (130)$$

Here we have

$$\begin{aligned} A &= \text{effective radius of mode 1} \\ B &= \text{effective variance} \\ C &= \text{effective radius of mode 2} \end{aligned}$$

NSD=3; Log-normal distribution

$$n(r) = \frac{1}{\sqrt{2\pi}\sigma_g} \frac{1}{r} \exp \left[-\frac{(\ln r - \ln r_g)^2}{2\sigma_g^2} \right] \quad (131)$$

where

$$\begin{aligned} A &= r_g \\ B &= \ln(\sigma_g) \end{aligned}$$

Table 17: A typical entry of *FJX_scat.dat*, where \bar{w}_0 is the single scattering albedo, and $w^1 - w^7$ are the terms 1–7 in the Legendre expansion of the phase function (the first term w_0 is always 1 and is omitted in the list).

| 15 S-Vol LOGN:r=.080 s=.800 n=1.514/.../1.435 reff=0.386 _ _ G=.0721_rho=1.630 |
|--|
| 200 2.5935 1.0000 2.092 2.914 2.880 3.295 3.185 3.430 3.379 |
| 300 2.6669 1.0000 2.121 2.861 2.792 2.936 2.733 2.703 2.568 |
| 400 2.5588 1.0000 2.144 2.813 2.711 2.695 2.425 2.257 2.069 |
| 600 2.1893 1.0000 2.149 2.713 2.547 2.362 2.018 1.740 1.499 |
| 999 1.4540 1.0000 2.118 2.537 2.277 1.951 1.555 1.229 0.972 |
| λ Q_{ext} \bar{w}_0 ω^1 ω^2 ω^3 ω^4 ω^5 ω^6 ω^7 |

Table 18: A typical entry of *mie.in*.

| |
|---|
| NSTEPS=04 NUMSD=01 NG=192IPART=10 NSIZEP=0 MIESPR=0 MIEOUT=3 SIZLIM=1.0D-09 |
| STEP= 0.05 FROM=00.00 TO= 2.00 |
| STEP= 0.10 FROM= 2.00 TO= 8.00 |
| STEP= 0.25 FROM= 8.00 TO=10.00 |
| STEP= 0.25 FROM=10.00 TO=90.00 |
| NSD=3 A= 0.080 B= 0.800 C= 0.000 RR1= 0.00 RR2= 2.50 |
| WAVL= 0.200 NR=1.460 NI=0.000 |
| WAVL= 0.300 NR=1.460 NI=0.000 |
| WAVL= 0.400 NR=1.460 NI=0.000 |
| WAVL= 0.600 NR=1.460 NI=0.000 |
| WAVL= 0.999 NR=1.460 NI=0.000 |

NSD=4; Power-law

For $a \neq 1$ we have

$$\begin{aligned}
 n(r) &= \frac{(a-1)r_1^{(a-1)}r_2^{(a-1)}}{r_2^{(a-1)} - r_1^{(a-1)}} r^{-a} \\
 &= \frac{1-a}{r_2^{(1-a)} - r_1^{(1-a)}} r^{-a} \quad \text{for } r_1 \leq r \leq r_2 \quad (132) \\
 &= 0 \quad \text{otherwise} \quad (133)
 \end{aligned}$$

and for $a = 1$

$$n(r) = \frac{r}{\ln r_2/r_1} \quad \text{for } r_1 \leq r \leq r_2 \quad (134)$$

$$= 0 \quad \text{otherwise} \quad (135)$$

where

$$\begin{aligned}
 A &= a \\
 C &= r_2 \\
 B &= r_1
 \end{aligned}$$

If you use the original program, you will have to hard-code the parameters and run the program for each wavelength you need.

The modified *spher_ctm3.f* loops over the wave lengths used in the Oslo CTM3, and may also loop over relative humidities.

RH-dependent or -independent

For RH-dependent aerosols, we set `LRHDEPENDENT=.true.`, otherwise to false. When `.true.`, the program will loop through RH from 0% with increments of 5.

If RH-dependent, look for results in *umdata.dat*, and for RH-independent in *scatdata.dat*.

What to change

Refractive indices are listed in `ASMRR` and `ASMRI`, and apply for wave lengths given in `ASLAM`. You have to define size distributions and how the radius grow due to RH. See the file to find out more.

12.5.2 Mishchenko *spher.f*

There are several codes for scattering available online at Mike Mishchenko's web page at GISS. His code for spherical aerosols is given in the *spher.f*, and is clearly based on the same source as `FJ_phase`, the work of Hansen and Travis (1974). This program is very well documented in the program file.

As already noted, you can find this code in the utilities of the SVN repository (Section B.1), and a modified version for the Oslo CTM3 can be found in the file *spher_ctm3.f*.

13 Sulphur module

The tropospheric sulphur chemistry is turned on by setting `SULPHUR :=Y` in the user specified section of *Makefile*. It is documented by Berglen et al. (2004).

To run this application you need to include at least the tropospheric chemistry module. The scheme needs 5 additional tracers, which are listed in Table 19. They need to be transported, and 4 of them are subject to wet deposition.

Table 19: The components of the sulphate application.

| Nr | Component name | Wet dep |
|----|--|---------|
| 71 | DMS (dimethyl-sulfide ^a) | Yes |
| 72 | SO ₂ | Yes |
| 73 | SO ₄ | Yes |
| 74 | H ₂ S | No |
| 75 | MSA (methanesulfonic acid ^b) | Yes |

^a(CH₃)₂S^bCH₃SO₃H

Originally two additional species included in the tracer array; CS₂ and OCS (carbonyl sulfide). However, they were calculated (no chemistry, no transport), so they are left out. They are not included because they are not important in the troposphere, but they do play a role in the stratosphere. When including sulphur chemistry in the stratosphere, these should be included.

13.1 Sulphur emissions

For SO₂ emissions it is usually assumed that 2.5% is emitted as sulphate, to account for oxidation. There are several datasets available for anthropogenic emissions. Biomass burning is usually from the Global Forest fires Emissions Database, with a vertical distribution from RETRO. Volcanic emissions are usually taken from AE-ROCOM or HTAP. Note that HTAP emissions are based on volcanic events, so make sure the emissions actually cover your simulation period.

No information is available on H₂S emissions from vegetation and soil, but they could be as described by Berglen et al. (2004).

DMS from ocean is parameterized as in Nightingale et al. (2000), where the DMS ocean concentration for each month is taken from Kettle and Andreae (2000), a climatology based on observations. The Kettle climatology for DMS was updated in 2010 by Lana et al. (2011), and this field is now also available. The updated climatology should be tested before it is used extensively. Also see Section 8.4.4.

In the Oslo CTM3 this climatology is given in the variable `DMSseaconc`, and is converted from units of nM (i.e. nmole/L) to kg/m. This is further converted to a flux using the parameterisation of Nightingale et al. (2000), based on wind speed from the meteorological data. The flux calculation is carried out in the `SOURCE` or `emis4chem` routine.

13.2 SO₄ scattering and absorption

Sulphate aerosols have optical properties that can be taken into account when calculating photochemical reaction rates.

Particles are assumed to be of log-normal size distribution, with dry radius of 0.05 μm and $\sigma = 2$, and will grow due to relative humidity according to Fitzgerald (1975).

Table 20: The components of the black carbon (BC) and organic matter (OM) application. All are transported. Wet scavenging is done for hydrophilic BC/OM, but also for 20% of hydrophobic BC aerosols on large scale ice precipitation. Most are numbered '1' to allow for more size bins or particle types.

| Nr | Component | Remarks |
|-----|-----------|------------------------------|
| 230 | omBB1fob | Insoluble OM biomass burn 1. |
| 231 | omBB1fil | Soluble OM biomass burn 1. |
| 232 | omFF1fob | Insoluble OM fossil fuel 1. |
| 233 | omFF1fil | Soluble OM fossil fuel 1. |
| 234 | omBF1fob | Insoluble OM biofuel 1. |
| 235 | omBF1fil | Soluble OM biofuel 1. |
| 236 | omOCNfob | Insoluble OM from ocean. |
| 237 | omOCNfil | Soluble OM from ocean. |
| 240 | bcBB1fob | Insoluble BC biomass burn 1. |
| 241 | bcBB1fil | Soluble BC biomass burn 1. |
| 242 | bcFF1fob | Insoluble BC fossil fuel 1. |
| 243 | bcFF1fil | Soluble BC fossil fuel 1. |
| 244 | bcBF1fob | Insoluble BC biofuel 1. |
| 245 | bcBF1fil | Soluble BC biofuel 1. |

Optical properties are found in *FJX_UMaer.dat*, in the entry `GM_S04`. Refractive indices used for calculating these data are for ammonium sulphate according to Toon et al. (1976), and the value at 200 nm is set to be equal to 300 nm, in lack of measurements below 300 nm.

14 Black carbon and organic matter

The black carbon and organic matter (BC/OM) application (Berntsen et al., 2006) is turned on by setting `BCOC :=Y` in the user specified section of *Makefile*.

This application is a stand-alone part of the Oslo CTM3 and needs the 14 tracers listed in Table 20.

Both water-soluble and insoluble species are emitted from different sources into the atmosphere (Section 14.1). The species are subject for deposition on the Earth surface (dry deposition, Section 14.2), and water soluble particles are also subject to wash-out.

Further, the insoluble species are transformed to soluble species after given *ageing times*. The ageing times are dependent on latitude and season, based on a simulation with the M7 application in the Oslo CTM2 (Skeie et al., 2011a; Lund and Berntsen, 2012). These are read from file in `bcoc_chetinit` in *bcoc_oslo.f90*, and stored in the array `CHET`. Input data is T42, which is interpolated to the model resolution.

BC can be deposited on snow, thereby changing the albedo of snow. A module for calculating BC on snow (Rypdal et al., 2009; Skeie et al., 2011a) is included in Oslo CTM3 (BCsnow, Section 14.5).

14.1 BC/OM emissions

The main sources of black carbon and organic matter comes from:

- Fossil fuel emissions
- Biofuel emissions
- Biomass burning

In addition, organic matter is emitted from the ocean, which is explained below.

Several datasets are available for the non-oceanic anthropogenic emissions, such as Bond et al. (2007). However, other inventories have recently become available, e.g. from the project ECLIPSE. Traditionally, fossil fuel and biofuel have been combined to one dataset, although recently it has become necessary to separate them.

Biomass burning is taken from Global Fire Emissions Database, which are distributed vertically according to the RETRO vertical distribution.

Organic matter released from the ocean follows Gantt et al. (2015), and is calculated in the file *emissions_ocean.f90*.

Important 1

The is method is based on sea spray production, but the Oslo CTM3 sea spray function is not necessarily the same as in Gantt et al. (2015). You should make sure the Oslo CTM3 does what you want it to.

If the SALT module (Section 16) is included, sea spray is retrieved from that module. If SALT is not included, sea salt production is calculated separately.

In the *emissions_ocean.f90* file, you can specify which sea spray scheme to use (parameter `SeaSaltScheme`; it may not be the same as used by the SALT module (it has a parameter with the same name)).

However, the actual schemes are listed in Section 16.1, and can be found in the file *seasaltprod.f90*.

Important 2

Note that when using ECLIPSE emissions, you have to turn off agricultural waste burning (AWB) in GFED. This is done by hard-coding the flags `partitions` in the GFED read-in routine *emisutils_oslo.f90*.

14.2 BC/OM deposition

All BC/OM tracers are dry deposited at the surface. The dry deposition velocities are simple; they consist of three constant values for each component, and applies for sea, land and ice. The land fraction controls when to use land or sea, while snow cover and ice cover (also sea ice) controls when to use deposition on ice. Generally the deposition rate is 0.025 cm/s, except for hydrophilic BC/OM over water, which is assumed to be 0.2 cm/s.

As for all Oslo CTM3 dry deposition velocities, these are modified due to the stability of the meteorological conditions. When deposited on the ground, the particles are lost to the model. However, the BCsnow module (if included) will keep track of the amount of BC deposited on snow (Section 14.5).

The hydrophilic aerosols are also washed out by rain, as will be described next.

14.3 BC/OM wet scavenging

BC and OM aerosols are scavenged by rain (Section 7.1), and as most aerosols they are assumed to be dissolved completely – i.e. mass limited removal. However, the removal on large scale ice precipitation is reduced, assuming that 20 % of the grid box is available for scavenging. The 20 % is somewhat arbitrary, but stems from the fact that these aerosols are scavenged by collision processes in rain, but in ice they are removed mainly by acting as ice nuclei (Browse et al., 2012). As will be explained below, we also apply the 20 % on large scale ice for hydrophobic BC/OC, and hydrophobic BC is also fully subject to convective wet scavenging.

Although Browse et al. (2012) suggested there should be no large scale wet scavenging for temperatures below 258 K, we also assume that 20 % of the grid box aerosols can be subject for large scale ice scavenging. Convective scavenging is assumed to be rain, having no such limit.

Most models seem to overestimate the stratospheric amount of BC, suggesting that tropospheric loss mechanisms are missing. Stratospheric loss processes are not very effective, covering gravitational settling and coagulation to mixed aerosols (e.g. together with sulphate).

As a possible tropospheric loss mechanism it has been suggested that hydrophobic BC is probably activated more quickly in convective rain, because of the large mixing going on within convective plumes. In principle there are two ways of parameterising this; either by calculating the aging time on-line, or to scavenge hydrophobic BC directly in convective rain.

We have chosen the second option, and we assume the wet scavenging to be similar to hydrophilic BC (but not for OM). The first option would require a microphysical parameterisation, and could in principle be taken from the M7 application not yet included in Oslo CTM3. Another possibility is to build a simpler scheme based on available model variables and tracers, such as sulphate and temperature. We have not yet looked into this.

14.4 BC/OM scattering and absorption

Black carbon (soot) and organic matter have some optical properties that can be taken into account. Properties depend on whether the aerosols are of fossil fuel origin (FF), biofuel (BF), or comes from biomass burning (BB).

BCFF

Dry aerosols, log-normal size distribution with radius 0.012 μm , standard deviation $\sigma = 2$. Refractive indices are from soot (World Climate Research Programme, 1986). Hydrophilic BCFF is assumed to have 50 % larger extinction coefficient, giving two entries in *FJX_scat.dat*: 31 `GM_BCFF_PHOB` and 32 `GM_BCFF_PHIL`.

BCBB and OCBB

Dry aerosols, bi-log-normal size distribution, with radii

$r_1 = 0.08$ and $r_2 = 0.16 \mu\text{m}$, standard deviations $\sigma_1 = 1.5$ and $\sigma_2 = 1.25$, and $\Gamma = 0.25/0.75$. Refractive indices are from the SAFARI campaign (Haywood et al., 2003b; Myhre et al., 2003a). Entry in *FJX_scat.dat* is 33 GM_BCOCBB

OCFF

Dependent on relative humidity. Log-normal size distribution with radius $0.5 \mu\text{m}$, and $\sigma = 2$. Refractive indices are from ammonium sulphate (Toon et al., 1976), and the value at 200 nm is set to be equal to 300 nm , in lack of measurements below 300 nm . Growth due to humidity follows Peng et al. (2001). Entry in *FJX_UMaer.dat* is labelled GM_OCFF.

14.5 BC on snow – BCsnow

The BCsnow module was first introduced by Rypdal et al. (2009) and later used by Skeie et al. (2011a). It diagnoses the amount of BC deposited on snow; it does not allow the deposited BC to get back into the atmosphere. When snow evaporates or melts, the BC is assumed to deposit on the ground and is thereby lost. Technically, it is a simple parameterisation for generating snow layers based on meteorological data, using snowfall and dry deposition values to account for the BC.

You turn this on by setting the logical parameter `LBCsnow=.true.` in *bcoc_oslo.f90*.

How it works

There are two processes depositing BC on snow: dry deposition and wet scavenging. During each operator split time step, dry deposition is diagnosed by the BCOM master routine (variables `bcsnow_dd_ffc`, `bcsnow_dd_bfc` and `bcsnow_dd_bio`), while a separate routine in `pmain` diagnoses wet scavenging based on the private arrays `BTT` and `BTTBCK` (variables `bcsnow_prec_ffc`, `bcsnow_prec_bfc` and `bcsnow_prec_bio`).

The parameter `ILMM` defines the maximum number of snow layers allowed. Snow is built in `BSNOWL`, while BC layers are built in `BBCFFC`, `BBCBFC` and `BBCBIO`. These four variables are of size `(ILMM, IDBLK, JDBLK, MPBLK)`.

When initializing from zero, the first snow layer is fetched from the meteorological data snow depth, but with maximum of 0.2 m water equivalents ($\approx 2 \text{ m}$ snow). Next, snow layers are produced by the amount of snowfall. This process is carried out after wet scavenging, by the BCsnow master routine `bcsnow_master`, before a few other processes/adjustments are taken into account:

- `bcsnow_collect_ij`: Collects BC deposited on snow.
- `bcsnow_evapmelt_ij`: Calculates evaporation and melting of snow.
- `bcsnow_seaice_ij`: Adjustment for sea ice.
- `bcsnow_adjustment_ij`: Other adjustments.

Collection

When BC is collected, it is always assumed that the uppermost layer is very thin (1 cm of snow, or 0.1 cm of water equivalents). This is to account for dry deposition being deposited only on the snow layer surface. If there is snowfall, both dry deposited and wet scavenged BC is first added to the uppermost thin layer. If there has been snowfall during the last 24 hours, the uppermost layer is

merged with the layer below, i.e. building a thicker layer. Finally, a new thin layer, with the same BC concentration, is made for the next round. Note, however, that the new thin layer is formed only if the current top layer is thicker than a threshold value, set to be 1.1 cm of snow. This is to avoid generating extremely thin layers.

Evaporation and melting

Evaporation and melting is treated as one process (sum of the meteorological fields). The levels below the topmost layer will be processed first, and when a layer is evaporated (fully or partially), its corresponding fraction of BC is merged with the topmost layer. The topmost layer is not affected until all layers below have disappeared.

Note that evaporation can be negative, and this is treated as extra snowfall, adding to the topmost snow layer.

Sea-ice treatment

The ECMWF meteorological data does not include snowdepth, snowmelt and evaporation on sea ice. We parameterise this as a linear reduction of the snow layer (on sea ice coverage larger than 30%) between spring and summer. Snow layers are not allowed if sea ice coverage is less than 30% .

Further adjustments

It may be that the snow layers generated from snowfall does not correspond fully with the snow depth given in the meteorological data. This is adjusted for here, but only for land surface, not for sea.

14.6 Secondary organic aerosols

Secondary organic aerosols (SOA) are part of the organic matter, and when running the stand-alone BCOM code, organic carbon may comprise both primary organic aerosols (POA or POM), and SOA. If, however, a more sophisticated SOA scheme is applied (see Section 19), the organic carbon species of the BCOM module act as POA only.

15 Mineral dust

The Dust Entrainment and Deposition (DEAD) Model (Zender et al., 2003) has been coupled to the Oslo CTM3. You include it by setting `DUST=:Y` in *Makefile*.

Based on wind and surface properties, it calculates the vertical (upward) flux of mineral dust (i.e. production), and based on observed size distributions (source modes) of mineral dust, the flux is distributed onto the model size bins. The DEAD module also calculates gravitational settling and deposition at the surface, although this can be implemented with other settling parameterisations. Washout is carried out in the Oslo CTM3 washout (see Section 15.4.2). It is, however, possible to let DEAD take care of washout, but this option is disabled in Oslo CTM3.

The DEAD code for the Oslo CTM3 is located in the directory *OSLO/DEAD_COLUMN*, and the DUST master routines connecting it to the Oslo CTM3 can be found in the master module *dust_oslo.f90* in *OSLO*. The original Oslo CTM2 files are located in the directory

OSLO/DEAD_COLUMN/dead_ctm2.

15.1 Get DUST running

The dust application can be run alone with two or more dust tracers. The number of tracers must be set in *cmn_size.F90* (NPART_DUST). Default is 8 tracers, as explained in Section 15.2.

DUST tracer names must be DUST01, DUST02, etc, and can be placed anywhere in the tracer list; they do not need to be listed after each other. But it is wise to declare them in increasing order, representing increasing size bins: The routines will not consider the numbering, but assign the first dust tracer to the smallest bin and the last to the largest bin. A separate array (*dust_trsp_idx*) keeps track of the transport numbers of the DUST species.

If you need to change the size distribution, see Section 15.2.

15.2 Dust size bins

In the standard set-up of Oslo CTM3, mineral dust is calculated using 8 size bins with diameters ranging logarithmically from 0.06 μm to 50 μm . The diameter size parameters are set in *dstpsd.F90*: *dmt_min* and *dmt_max*.

The dust source is controlled by the observed source modes described next. In principle, it should not be necessary to change the size range, and probably not the number of bins. If you want to do changes to the model size bins, this is done in *cmn_size.F90* (NPART_DUST). You also have to change the properties used in fast-JX.

15.3 Dust sources

Mineral dust is produced by wind blowing across surfaces where mineral dust occur. Information on earth surface is read from the DUST input file *dst_Txxx.nc*, and the user can select a mobilisation map and a matching scaling factor. This is described in Section 15.3.1 for more.

How the production is technically done, is described in Section 15.3.2.

DEAD can use mean winds or it can use a probability density function for wind speed. This treatment is discussed in Section 15.3.3.

15.3.1 Input files needed

DEAD reads time invariant (static) and time variant surface fields from the file *dst_Txxx.nc*, where *xxx* should match the native metadata resolution (only either T159 or T42 are available). The files are located in the directory *OSLO/DEAD_COLUMN/dustinput*, and you need to copy the correct file to the directory where you run the model.

Such input files can be generated with the *map* module written by Charlie, see Appendix C.5 for more on *map*.

Table 22: Mobilisation dataset and fudge factors: Your choices must be set in *Ltracer_emis_xxxx.inp*, and it is important that the fudge factor matches the mobilisation dataset. The factors were made for Oslo CTM2, and are to some extent resolution dependent, so you have to check the annual total production to find the correct factor for your runs.

| Mobilisation dataset | fudge factor |
|--------------------------|-------------------------|
| bsn_mds_sqr (pdf winds) | 1.4686×10^{-4} |
| bsn_mds_lnr (pdf winds) | 1.0780×10^{-4} |
| bsn_mds_lnr (mean winds) | 2.5046×10^{-4} |
| mb1_bsn_fct (pdf winds) | 2.1994×10^{-4} |
| area_acm_fct (pdf winds) | N/A |

Note that this program has not been compiled and used since around 2005.

Mobilisation/erodibility dataset

Several fields are read from *dst_Txxx.nc*, but there is only one field where the user can make a choice, namely which mobilisation dataset/map to read. This field is also referred as the *erodibility* or *erodibility factor*.

There are several erodibility maps available, as listed in the left column of Table 22, but not all should be used. The standard field for Oslo CTM3 should be *bsn_mds_sqr*, as found by Grini et al. (2005), but it seems Oslo CTM2 has used *mb1_bsn_fct* ever since, which is what Oslo CTM3 has inherited.

It should be noted that in the DEAD code, the erodibility map is called *mb1_bsn_fct* (file *dsttidbs.F90*), even though another map is used. This is somewhat unfortunate, but I didn't want to change the variable names in *dst_Txxx.nc*.

Fudge factor

In addition, the user must define a global scaling factor (fudge factor) that should match the mobilisation dataset. You specify this with the EFAC number in the STV section of *Ltracer_emis_xxxx.inp*, as shown in Table 21.

The fudge factor is used to scale dust production up or down, to get a certain annual total of emissions. The fudge factor is somewhat resolution dependent, so you need to make sure you use the correct value (check annual total production). What you specify for EFAC in the STV section of *Ltracer_emis_xxxx.inp*, is stored in *flx_mss_fdg_fct0* in *dstcst.F90*, and used later in *dstmb1.F90*.

Note that the fudge factors are not well tested in Oslo CTM3, and if 'N/A' is listed in Table 22, you should use it with care.

15.3.2 Technical

DEAD calculates first the horizontal flux of mineral dust, which is not what is transported horizontally in the model, but the basis for calculating the vertical flux, i.e. the mobilisation of dust. From observed source size modes of dust, the vertical flux is next partitioned

Table 21: Defining fudge factor and mobilisation dataset in the STV section of *Ltracer_emis_xxx.inp*.

| | | | | | | | | | |
|---|--|-----|----|------|-----|---|----|---|---------------|
| 'DEAD_Mineral_Dust_FudgeFactor_and_Mobilisation_Dataset_Name' | | | | | | | | | |
| 556 | 1.4686d-04 | HLF | 99 | 9999 | NAT | 0 | -1 | 0 | 'bsn_mds_sqr' |
| --- | #This section sets mobilisation map name and fudge factor for DUST | | | | | | | | |

into the model size bins, using the overlap fraction `ovr_src_snk_frc`, i.e. the fraction of each source mode going into each model size bin.

There are currently 3 source modes (`dst_src_nbr` in *dstgrd.F90*), given by parameters in the routine `dst_psd_src_ini` in *dstpsd.F90*:

- `mss_frc_srcx`: Mass fraction.
- `dmt_vma_srcx`: Mass median diameter [m].
- `gsd_anl_srcx`: Geometric standard deviation.

These are the parameters you need to change if you want a different size distribution of the emissions.

The overlap fraction is thus a matrix of size (`dst_src_nbr`, `DST_NBR`), giving the fraction of size distribution i in source modes that overlap with model bin j .

There are two methods available for calculating the fluxes:

- 1 Horizontal flux from White (1979) in subroutine `flx_mss_hrz_slt_ttl_Whi79_get` in *dstmblutl.F90*. Vertical flux from Marticorena and Bergametti (1995) in routine `flx_mss_vrt_dst_ttl_MaB95_get` (same file).
- 2 Follows Alfaro and Gomes (2001). **Should be checked against a more recent version of DEAD before use.**

Option 1 is default, and to use Option 2 you have to include the appropriate DUST token (`ALG01`) in *Makefile*.

Depending on your bins and distributions, the model bins may or may not cover all sizes given by the defined source bins. If the i -th source is completely bracketed by model bins, then

$$\sum_{j=1}^{j=\text{dst_nbr}} \text{ovr_src_snk_frc}(i, j) = 1 \quad (136)$$

and similarly, if the j -th model bin completely brackets the sources, then:

$$\sum_{i=1}^{i=\text{dst_src_nbr}} \text{ovr_src_snk_frc}(i, j) = 1 \quad (137)$$

The part of the sources bins being smaller or larger than the model size bin range will not be accounted for.

Note that inputs for calculating the overlap fraction are generic median diameters of lognormal distributions. Thus, if the routine is called with number median diameters it will compute the overlap factors for number concentration, and if it is called with mass median diameters then it will compute the overlap factors for mass.

For the default Option 1, this is done in `ovr_src_snk_frc_get` in *psdlgn.F90*, called from `dst_psd_ini` in *dstpsd.F90*. This fraction is converted

to mass (`ovr_src_snk_mss`). If you use Option 2, the overlap (`ovr_src_snk_mss`) is updated each time step in `dst_mbl` in *dstmbl.F90*.

Scaling the fluxes

After horizontal fluxes are calculated, they are scaled linearly with:

- Bare ground fraction.
- Erodibility map/mobilisation factor.
- Fudge factor.

15.3.3 Wind speed variability

Dust is formed due to wind at the surface, and although the grid box wind is given from the meteorological data, the actual wind will vary around the mean wind. Because the dust production is sensitive to the wind speed, the inclusion of wind speed variability may be important. By default we apply a variability of 5 steps (parameter `wnd_mdp_nbr` in *dstmbl.F90*), so that the calculation of dust production (i.e. the flux from the surface) is done for 5 wind speeds; the mean wind, two lower and two higher wind speeds, before being weighted properly to form the total dust flux.

For a grid value of 10 m/s and `wnd_mdp_nbr`=5, the dust flux will be calculated for winds of approximately 6, 8, 10, 12 and 14 m/s, and then weighted to one flux.

You can turn this off by setting the variable `wnd_mdp_nbr`=1 in *dstmbl.F90*. It is also possible to increase this number.

15.4 Dust sinks

Mineral dust can be removed by precipitation and by gravitational settling.

15.4.1 Gravitational settling

Currently, DEAD handles the gravitational settling, but this should probably be revised when a second order moment routine is available. The fall velocity is calculated from Stokes theory, and at the surface the velocity is adjusted due to turbulent mixing.

15.4.2 Wet scavenging

Dust tracers are washed out as regular tracers, following the parameters listed in the file *scavenging_wet.dat*. All dust tracers are assumed to be soluble, as they generally are good cloud condensation nuclei. They are also removed by ice.

If you include more DUST tracers, make sure they are defined to be wet scavenged in the file *scavenging_wet.dat*.

15.5 DUST scattering and absorption

Mineral dust have optical properties that can be taken into account when calculating photochemical reaction rates.

The dust bins (8 by default) are assumed to logarithmically span the diameter range of $0.06\text{ }\mu\text{m}$ to $50\text{ }\mu\text{m}$, so that the size of aerosols in each bin are monodisperse (no variation of diameter in each bin). However, within each bin, the mass weighted diameter is calculated, based on the bin sizes and mass median diameter (`dmt_vma` in routine `dst_psd_ini` in *dstpsd.F90*) and standard deviation of the distribution (`gsd_anl`, same location). Default value for `dmt_vma` is $2.524\text{ }\mu\text{m}$, with a standard deviation `gsd_anl` of 2. These numbers are supposedly taken from Shettle (1984), but I could not manage to find it. Zender has probably a copy if you need it.

Particle density is assumed to be 2.6 g/cm^3 , and refractive indices are taken from the SHADE campaign (Haywood et al., 2003a; Myhre et al., 2003b).

Mineral dust does not swell with increased humidity, so the scattering and absorbing properties are listed in the file *FJX_scat.dat*, having entries `GM_DUST1` to `GM_DUST8`.

Important

If you change either the size of the bins, or the mass median diameter (`dmt_vma`) or standard deviation (`gsd_anl_dfl`), you have to re-compute the table values for `GM_DUST` in *FJX_scat.dat*.

15.6 Things to watch out for

Oslo CTM3 and DEAD are since 2015 fully consistent in resolution parameters.

Note that DEAD has level 1 on the top (i.e. the top of the atmosphere has index 1). The transformation is taken care of in the subroutines in *dust_oslo.f90*.

In the DEAD file *blmutl.F90* two fixes have been added. The first is to make sure the displacement height is never higher than 70 % of the midpoint height. The second is to make sure that roughness height is never higher than 70 cm, which seemed to give problems in iterations for some grid points at some specific times (that is: the energy budget for the first layer did not converge).

15.7 Dust budgets

The dust module outputs a file called *ctm3dstbudget.nc* which is the budget for dust. The file contains 5 temporally averaged fields, which are average fluxes ($\text{kg/m}^2/\text{s}$) of dust for different processes, and one average for the burden (kg/m^2):

- Convective wet deposition [$\text{kg/m}^2/\text{s}$]
- Large scale wet deposition [$\text{kg/m}^2/\text{s}$]
- Dry deposition [$\text{kg/m}^2/\text{s}$]
- Production [$\text{kg/m}^2/\text{s}$]

- Total burden [kg/m^2]

The time span for the average is defined as for the SALT module; using the core budget tendencies calendar (“BUDGET tendencies calendar” flags in *LxxCTM.inp*). Also grid area is put out.

By default, the budget terms are summed up over all dust tracers, but you can also put out budget terms for each of the tracers. The latter is done by setting `LDUSTDIAG3D=.true` in *dust_oslo.f90*.

3D averages of dust mass is put out as usual by the core diagnostics. For dust, it makes more sense to talk about mass mixing ratio (kg/kg) since the dust is not molecules as such.

15.8 Additional notes

The original DEAD model available from Zender was coded to be parallelized over latitudes, and had to be re-structured for the column treatment in Oslo CTM3; to run the original DEAD model as a column model (with parameters `PLON=PLAT=1`) does not fit the treatment of input data for a global model. So the code was re-organized to yield a purely column treatment.

Important

If you include more DUST tracers, make sure they are defined to be wet scavenged in the file *scavenging_wet.dat*.

The DEAD version implemented is 1.3.2. There are, however, newer versions available; check the web site⁴ for information. If an update is needed, check the new version against the code we use. Be certain that you keep the column treatment of the Oslo CTM3; if necessary, you can compare the new version to the old code in *OSLO/DEAD_COLUMN/dead_ctm2*.

15.9 Into the future

The DEAD model included should be updated to a more recent version.

16 Sea salt

The sea salt application was introduced by Grini et al. (2002). It is an independent application which can be included in any transport model.

In the Oslo CTM3, the salt code is located in the file *seasalt.f90*. It is primarily based on Fitzgerald (1975).

Sea salt production, however, is located in a separate module *seasaltprod.f90*, because it is used to calculate emissions of organic matter from ocean.

⁴<http://dust.ess.uci.edu/dead/>

16.1 Sea salt production

The sea salt production, or flux, is found in the array `seasalt_flux`, and is of size (NPAR_SALT, IDBLK, JDBLK, MPBLK) and has units kg/s.

The flux is calculated from the winds, and hence carried out every meteorological time step, by the subroutine `seasalt_emis`. Several methods are available, set by `SeaSaltScheme` in `seasalt.f90`:

- 1 Monahan et al. (1986) for small particles, as suggested by Gong et al. (1997), and Smith et al. (1993) for large particles. This is the default heritage from Oslo CTM2.
- 2 Mårtensson et al. (2003).
- 3 Gantt et al. (2015), i.e. Gong (2003) with sea surface temperature adjustment as in Jaeglé et al. (2011).
- 4 Witek et al. (2016), i.e. Sofiev et al. (2011) without salinity effects, using sea surface temperature adjustment as in Jaeglé et al. (2011).

Seasalt flux is used to calculate emissions of organic matter from ocean, in `emissions_ocean.f90`. Also see Section 14.1 for some more info.

16.2 Technical information

The salt aerosols are divided into bins, and there is one tracer field for each bin. The tracer names are SALT01, SALT02, etc. They do not need to be listed after each other, but should be (it is wise to keep the tracers close to each other in the transport array). The tracers should be listed in increasing order (01, 02, 03, ...) since the size bins will be assigned from small to large, using the names encountered in the tracer list.

The QSSA solver is used to integrate sea salt (for each bin). The production terms are surface emissions (only in the lowermost layer) and gravitational settling from the layer above (except for the top layer). The loss term includes gravitational settling to layers below (all layers except lowest layer) and dry deposition (lowest layer). Hence surface layer dry deposition differs from gravitational settling.

So far the emissions and dry deposition are treated as production and loss terms in the QSSA solver. *This may be non-compatible with the UCI emission treatment, and may need to be revised.*

Water makes the sea salt particles grow to larger sizes. However, this water is not transported. The growth is calculated locally each timestep, depending on the local relative humidity, and the information on how large the aerosols are are used to adjust their falling velocity and their dry deposition velocity.

16.2.1 Wet scavenging

Sea salt aerosols are assumed to be absolutely soluble and are removed in the convective and stratiform precipitation processes in the Oslo CTM3. Wet scavenging parameters are set in the file `scavenging_wet.dat`.

Important

If you include more SALT tracers, make sure they are defined to be wet scavenged in the file `scavenging_wet.dat`.

16.3 SALT scattering and absorption

Sea salt have optical properties that can be taken into account when calculating photochemical reaction rates.

For dry aerosols, the 8 size bins are assumed to logarithmically span the diameter range of $0.03\ \mu\text{m}$ to $25\ \mu\text{m}$, so that the size of aerosols in each bin are monodisperse (no variation of diameter in each bin).

Salt particles will grow due to relative humidity, and optical properties are found in `FJX_UMaer.dat`, where the entries are GM_SALT1 to GM_SALT8. The growth follows Fitzgerald (1975), and refractive indices used for calculating these data are taken from Shettle and Fenn (1979) and Rothman et al. (2003).

16.4 Salt budgets

The SALT module produces averages of the salt budget, on the same days as the core budget tendencies does; it uses the “BUDGET tendencies calendar” flags in `LxxCTM.inp`. The routine is called from pmain after core tendencies have been processed, and the netCDF output file is called `ctm3sltbudget.nc`.

Several processes are diagnosed:

- Production [$\text{kg}/\text{m}^2/\text{s}$]
- Dry deposition [$\text{kg}/\text{m}^2/\text{s}$]
- Large scale wet deposition [$\text{kg}/\text{m}^2/\text{s}$]
- Total burden [kg/m^2]
- Convective wet deposition [$\text{kg}/\text{m}^2/\text{s}$]

By default, the budget terms are summed up over all sea salt tracers, but you can also put out budget terms for each of the tracers. The latter is done by setting `LSALTDIAG3D=.true` in `seasalt.f90`.

In the netCDF file you find all the information you need, including grid area, the time span of accumulation, etc.

17 Nitrate

Aerosol nitrate can be simulated with the equilibrium module developed by Metzger et al. (2002). In the Oslo CTM3 it needs to be run together with tropospheric chemistry (Section 10), sulphate module (Section 13) and the SALT module (Section 16). These must be turned on in the user section in `Makefile`.

The nitrate master routine is located in the file `nitrate_oslo.f90`, and it works on IJ-blocks, calling the Metzger program as a column model.

Note that the nitrate module is not used in the stratosphere. When stratospheric chemistry is included, the nitrate module is applied up to the tropopause height (`maxval(LMTROP(I,J))`). When stratospheric chemistry is turned off, nitrate is calculated up

to the maximum tropopause height of the latitude band (`maxval(LMTROP(:, J))`) plus a few layers (`LVS2ADD2TC`).

In the stratosphere nitrate species are converted to HNO_3 , and therefore also added to NO_y . This stratospheric loss was not included in CTM2.

The Metzger program takes into account sulphate, total HNO_3 (i.e. $\text{HNO}_3(\text{gas}) + \text{NO}_3(\text{aerosol})$), total NH_3 (i.e. $\text{NH}_3(\text{gas}) + \text{NH}_4(\text{aerosol})$). The basic principles for gas/aerosol partitioning in Metzger's program are:

- All sulphate exists as aerosols.
- The most stable form of sulphate is Na_2SO_4 .
- The next most stable form of sulphate is $(\text{NH}_4)_2\text{SO}_4$.
- The most stable form of aerosol ammonium is $(\text{NH}_4)_2\text{SO}_4$.
- Nitrate can exist in aerosols if neutralized by NH_3 .
- Nitrate only exists in aerosols if it is cold (due to the Clausius Clapeyron equation).

17.1 Nitrate physics – modes

In nature, condensation/evaporation drives the partitioning of HNO_3 . In the equilibrium-module, however, there is no way to follow the path from gas to aerosol. What is found is the partitioning with lowest Gibbs energy of the mixture we put in.

The equilibrium routine will predict Na_2SO_4 aerosols if both Na^+ and SO_4^{2-} are in the mixture. However, since both SO_4^{2-} and Na^+ are non-volatile, given a mixture of NaCl , H_2SO_4 , HNO_3 and NH_3 the equilibrium model could predict aerosol Na_2SO_4 and otherwise gaseous components.

However, if sulphates are small aerosols (accumulation mode) and NaCl are large aerosols (coarse mode), the only way Na can mix with SO_4 is through coagulation and not through condensation.

To treat this right, we make the (simple) assumption that sulphate exists as a “fine” mode, and sea salt as a “coarse” mode. We calculate chemical equilibrium for both modes.

For the first mode, we calculate chemical equilibrium for the mixture of NH_3 , HNO_3 and H_2SO_4 , which will normally predict aerosol $(\text{NH}_4)_2\text{SO}_4$. If any excess NH_3 is present and if it is cold enough, aerosol NH_4NO_3 will be predicted.

For the coarse mode, equilibrium between the leftover from the first equilibrium (HNO_3 and NH_3) and NaCl is calculated. Normally this will transfer a large part of HNO_3 to the aerosol phase, creating NaNO_3 . The “small” mode should have the chance to reach equilibrium first; because of their higher surface to mass ratio, they reach equilibrium much quicker than the larger ones.

To make things simple, aerosols are assumed meta-stable in the Oslo CTM3, so that we don't need to take into account particle history.

17.2 Nitrate tracers

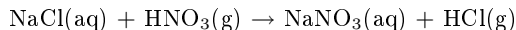
As noted, the nitrate application depends on tropospheric chemistry, sulphate and sea salt applications. The new tracers needed for this simulation are given in Table 23. Wet scavenging of NH_3 is based on Henry's law, assumed not to be taken up in ice, while the aerosols are assumed to be mass limited uptake (see Section 7.1.1).

$\text{H}_2\text{O}_{\text{fine}}$ and $\text{H}_2\text{O}_{\text{coarse}}$ are not used in the Oslo CTM3, since H_2O is not transported. They are only used as diagnostics, and are therefore left out until transport is necessary; they are calculated privately in the nitrate module *nitrate_oslo.f90*.

17.3 Sea salt in the nitrate model

Sea salt is crucial to the nitrate application. The standalone sea salt application is treated in mass space and does not need a specific molar mass. However, when nitrate is included it is important that you put the correct molecular mass to the sea salt tracers (which is 58 g/mol), because the equilibrium model evaluates how much of the Cl in NaCl which can be replaced with NO_3 .

Note that after this has been evaluated, sea salt is transported as NaCl again. This might seem inconsistent since strictly speaking, they may contain some NaNO_3 . However, this is not important since NaNO_3 is more stable than NaCl and if we have NO_3^- available it will replace the Cl^- in the next timestep also. The reaction happening is:



However, the fact that we set $[\text{Cl}^-] = [\text{Na}^+]$ as input to the equilibrium calculations does not really change the output since HCl is the first gas to evaporate anyway. If HNO_3 is available, it will replace Cl^- until $[\text{NO}_3^-] = [\text{Na}^+]$. Thus the important thing is to keep track of Na^+ , which we do in the sea salt tracers.

17.4 Nitrate emissions

The nitrate application needs emissions of NH_3 . Different datasets are available, e.g. GEIA (Bouwman et al., 1997) which has traditionally been used in Oslo CTM2. However, newer sets are also available, e.g. from Lamarque et al. (2010). While the latter covers only anthropogenic emissions, the GEIA data covers both anthropogenic and natural emissions, given on 1x1 resolution on an annual basis. Following Adams et al. (1999), we impose a monthly variation on three datasets by weighting emissions by the number of daylight hours during the year: Domestic animals, fertilizers, and crops sources.

The GEIA dataset is rather old, so it should probably be updated.

The Oslo CTM2 emissions were summed up in one file, which made them less flexible. Therefore, the format is updated, and the GEIA datasets are available on a netCDF file, scaled to $\text{kg}(\text{NH}_3)/\text{s}$ for 12 months. Three of them are scaled with sunlit hours as described above.

Table 23: Tracers included in the nitrate model. H2Ofine and H2Ocoarse are only used in diagnostics, and are therefore left out until transport is necessary; they are calculated privately in the nitrate module.

| Nr | Component name | Remarks | Approximate lifetime | Transport | Wet dep. |
|----|----------------|---|----------------------|-----------|----------|
| 61 | NH3 | Gas, emitted | weeks | Yes | Yes |
| 62 | NH4fine | | weeks | Yes | Yes |
| 63 | NH4coarse | | days | Yes | Yes |
| 64 | NO3fine | | weeks | Yes | Yes |
| 65 | NO3coarse | | days | Yes | Yes |
| – | H2Ofine | Aerosol water adjusts rapidly to ambient RH | short | — | — |
| – | H2Ocoarse | | short | — | — |

All original files are available in `/div/amoc/d4-4/oslo-ctm/archive_ctm/input_files/`, in the subdirectory `emissions/NH3_GEIA`. Here you also find the program `sum_data_as.f`, which does the scalings (the original file scaled all datasets with sunlit hours). While producing monthly totals in separate files, it also produces a file that the IDL program `make_geia_netcdf.pro` uses to make the netCDF file.

Emissions files can be found in the emission directories, and must be included in the emission list `Ltracer_emis_XXX.inp`.

17.5 Remaining problems

The dry deposition of NH₃ is set to some numbers found in an old paper by Sorteberg and Hov (1996). There seems to be agreement that drydep velocities of NH₃ should exceed velocities of NH₄⁺, but it is unclear by how much. The new dry deposition scheme (Section 7.2) may improve this.

Based on the first nitrate studies with Oslo CTM2, it seems that the amount of NO₃ fine aerosol is heavily dependent on how efficiently NH₃ is mixed up to altitudes where it is cold enough to form NH₄NO₃. At ground it is usually quite warm, while at higher altitudes aqueous production of H₂SO₄ makes aerosols too acidic to form NH₄NO₃.

A scientific analysis of the Oslo CTM3 should perhaps include sensitivity to vertical mixing, since the first CTM2 results seem to indicate that NH₃/NH₄⁺ is not mixed to cold enough layers, and the cold layers thus stay acidic due to high sulphate production there.

17.6 Box version

A box version of the nitrate code exists in the Oslo CTM3 tool box at `/div/amoc/d4-4/oslo-ctm/archive_ctm/box_models/`.

18 M7

M7 is not yet implemented, and there is no plan yet to do so.

19 Secondary organic aerosols (SOA)

Secondary organic aerosols (SOA) was implemented in Oslo CTM2 by Hoyle et al. (2007), and utilised later in e.g. Hoyle et al. (2009a).

Several precursor hydrocarbons are included (Section 19.1). The precursors also react within the tropospheric gas phase chemistry, oxidised by OH, O₃ and NO₃, forming SOA gas phase components (Section 19.2). A separate module calculates SOA from an equilibrium approach, as explained in Hoyle et al. (2007).

Stoichiometric coefficients are used for the chemical products, based on a two-product model (Hoffmann et al., 1997), and the partitioning (or separation) between the gas and aerosol phases is calculated assuming equilibrium and using partitioning coefficients (Hoyle et al., 2007).

Importantly, in Oslo CTM3 we do the separation in both the troposphere and the stratosphere, but the chemical conversion from precursors is only carried out in the troposphere. Stratospheric separation was not treated in Oslo CTM2.

19.1 SOA precursor tracers

The SOA precursor VOCs are listed in Table 24. In addition, the Oslo CTM3 component **C6HXR** has been split in three, namely **C6HXR_SOA** for trimethyl-benzenes, **Benzene** for benzene and **Tolmatic** for toluene and other aromatics.

19.2 SOA tracers

The SOA tracers are several gas components **SOAGAS_{xy}**, where **x** is the class number (1–8), and **y** is the oxidising component (1–3, O₃, OH, NO₃). Similarly, there are aerosol components **SOAAER_{xy}**. These components have component IDs between 150 and 191. See Hoyle et al. (2007) for more information.

19.3 SOA sources and sinks

The SOA precursors are emitted from the earth surface, using a rather old dataset, which should be updated. These precursors, and also isoprene, are emitted assuming emissions only at daytime and scaled to sunlight, as described in Section 8.4.4.

SOA are produced or lost according to the separation method, which is based on temperature; i.e. the separation can be either production or loss.

SOA gases and the precursor gases are assumed to have a stratospheric lifetime of 1 month, assuming the SOA are converted into species not treated in the model. Oslo CTM2 used a lifetime of 1 week, which was considered too short and hence upped in Oslo CTM3. See *strat_loss.f90* for more. SOA aerosols are subject to gravitational settling (also treated in *stratloss_loss.f90*), and if you run the Oslo CTM3 without stratospheric chemistry, the 1 month lifetime also applies for the aerosols.

20 Physics

Based on the meteorological data, some physical properties may be calculated. These include tropopause height, equivalent latitude, potential vorticity, etc. The physics routines are located in the physics module, which can be found in the file *physics_oslo.f90* in the *OSLO* directory. Also see Appendix C, where e.g. air mass, layer thickness and relative humidity is calculated.

20.1 Tropopause height

In Oslo CTM3, several routines need to distinguish between tropospheric and stratospheric air. This is

Table 24: The secondary organic aerosol precursor components. Bottom three replaces the usual C6HXR in Oslo CTM3.

| Nr | Component | Remarks |
|-----|-----------|--|
| 280 | Apine | α -Pinene |
| 281 | Bpine | β -Pinene |
| 282 | Limon | Limonene |
| 283 | Myrcene | Myrcene |
| 284 | Sabine | Sabinene |
| 285 | D3carene | Δ^3 -Carene |
| 286 | Ocimene | Ocimene |
| 287 | Trpolene | Terpinolene |
| 288 | Trpinene | α - and γ -Terpinene |
| 289 | TrpAlc | Terpinoid alcohols |
| 290 | Sestrp | Sesquiterpenes |
| 291 | Trp_Ket | Terpenoid ketones |
| 192 | Benzene | Benzene |
| 193 | Tolmatic | Toluene and other aromatics |
| 12 | C6HXR_SOA | Trimethyl-benzenes and xylene (replaces C6HXR) |

typically done by finding the tropopause, which is 2-dimensional, or it can be done in 3D.

The chemistry is so far set up to use a 2D tropopause to select when to use the tropospheric module and when to use the stratospheric module. Some diagnostics such as STE flux uses 3D fields to separate tropospheric from stratospheric air.

In any case there are several ways to calculate the tropopause. The 3D representation is explained in Section 21.1.4, while the 2D representation is described here. As noted above, the routine can be found in the file *physics_oslo.f90*.

What we call the tropopause (2D) is defined as the uppermost layer of the troposphere, and is therefore named **LMTROP** (historically, LM was often used as parameter instead of LPAR).

20.1.1 PVU based tropopause

First, the tropopause level is not allowed to have potential temperature higher than 380 K (Holton et al., 1995). The uppermost layer having potential temperature below 380 K is called **L380K**.

Traversing downwards from **L380K**, the tropopause (top layer of troposphere) is defined at the level where the PVU (10^6 PV) is lower than 2.5 PVU (Holton et al., 1995), but not lower than 5 km (a somewhat arbitrary value, not often encountered). If the maximum PVU is lower than this limit (typical for low latitudes) the tropopause is defined at **L380K**; the upper-most level where potential temperature is lower than 380 K.

Sometimes the minimum (absolute value) PVU in a column can be greater than 2.5 (e.g. in the polar vortex). In that case, two options remains; if there exists an altitude of minimum absolute PVU, it is chosen as tropopause. If PVU decrease monotonically with depth (i.e. downwards), the tropopause is set to a default minimum height of 5 km.

The routine is called **tp_pvu_ij** and you set this option using **TP_TYPE=1** in *cmn_oslo.f90*.

20.1.2 Lapse rate based tropopause

The tropopause can also be found traversing upwards until the level where the lapse rate (calculated between the current level and the next)

$$-dT/dz = -\frac{T_{L+1} - T_L}{z_{L+1} - z_L} \quad (138)$$

goes below 2 K/km.

It assumes a minimum tropopause height of 5 km, and a maximum height given by 50 hpa (top of grid box must have larger pressure than this).

The routine is called **tp_dtdz_ij**, and you set this option using **TP_TYPE=2** in *cmn_oslo.f90*.

20.1.3 Lapse rate based on E90 tracer

The tropopause defined by the E90 tracer (Prather et al., 2011) can be used if the E90 tracer is included. It is the uppermost level where the 3D LSTRATAIR_E90 is `.false.` (i.e. tropospheric air), as given by the variable LPAUZZTOP.

The routine is called `tp_e90_ij`, and you set this option using `TP_TYPE=3` in `cmn_oslo.f90`.

20.2 Potential vorticity

Potential vorticity (PV) is available in the L60 meteorological data, but only in a few L40 data sets. If not available, PV will be calculated from the meteorological data (temperature, wind and pressure). A routine for this is available in `physics_oslo.f90`.

20.3 Equivalent latitude

In the physics module (in the file `physics_oslo.f90`) we also calculate equivalent latitude. Equivalent latitude is calculated from PVU according to Nash et al. (1996), based upon the fact that PV is assumed to be conserved on potential temperature (θ) surfaces. All necessary parameters and variables are defined in the physics module.

How it is done

We define NTHE θ levels in the parameter `pvthe(NTHE)`, and we interpolate PV onto each of those levels. Then we find equivalent latitudes for all horizontal grid boxes for those θ surfaces.

The calculation of equivalent latitude is carried out for each hemisphere separately. Max absolute PV is in the polar vortex, and is therefore assumed to be the pole in equivalent latitudes. Minimum is at Equator. The PV span is divided into bins, and the area covering each binned value of PV is calculated. Depending on the area containing each PV, each grid box is assigned an equivalent latitude. See the routine for equations and description.

Remember that equivalent latitude is only useful in the uppermost troposphere and in the stratosphere, which should be reflected in the `pvthe` values.

How to use the data

For a given grid box, find the potential temperature and interpolate equivalent latitude from the closest θ levels in `pvthe`.

20.4 Boundary layer height

The routine `set_blh_ij` sets BLH from the boundary layer height at the current and next meteorological time step (BLH_CUR and BLH_NEXT, respectively). This is interpolated linearly in time, and we interpolate halfway into the time step Δt_{chem2} of the CCYC-loop. The weighting fraction of current and next fields are then

$$f_{\text{next}} = \frac{\text{nmetTimeIntegrated} + \frac{\Delta t_{\text{chem2}}}{2}}{\Delta t_{\text{met}}} \quad (139)$$

$$f_{\text{cur}} = 1 - f_{\text{next}} \quad (140)$$

where `nmetTimeIntegrated` is the elapsed time of the meteorological time step, and Δt_{met} is the meteorological time step.

For diagnostic output which are done every NOPS, the weighting is done to get BLH at each NOPS:

$$f_{\text{next}} = \frac{\text{NOPS} - 1}{\text{NROPSM}} \quad (141)$$

$$f_{\text{cur}} = 1 - f_{\text{next}} \quad (142)$$

Both BLH_CUR and BLH_NEXT needs to be set when reading meteorological data. If BLH_NEXT cannot be found, it should be set to the same as BLH_CUR.

20.5 Land surface types

The Oslo CTM3 needs information about land surface types, also called land use types or pland functional types (PFT). These are used e.g. for dry deposition scheme or in the biogenic emission routines.

Prior to the inclusion of online biogenic emissions (see Section 8.6), a MODIS dataset was used. Now we use the PFT field from the Community Land Model (CLM), giving vegetation information for 16 types for all years since 1860. Specifics of the PFTs are listed in Table 25 and Table 26.

The land surface type fractions for a grid point I,J are stored in `landSurfTypeFrac(:,I,J)`. You define which year to apply in the input file, stored in `LANDUSE_YEAR`. If you set 9999, the meteorological year will be used. The variable `LANDUSE_IDX` sets the dataset you want, 2 is MODIS and 3 is CLM.

Table 25: CLM-PFTs.

| # | Name |
|----|-------------------------------------|
| 1 | Needleaf evergreen temperate tree |
| 2 | Needleaf evergreen boreal tree |
| 3 | Needleaf deciduous boreal tree |
| 4 | Broadleaf evergreen tropical tree |
| 5 | Broadleaf evergreen temperate tree |
| 6 | Broadleaf deciduous tropical tree |
| 7 | Broadleaf deciduous temperate tree |
| 8 | Broadleaf deciduous boreal tree |
| 9 | Broadleaf evergreen temperate shrub |
| 10 | Broadleaf deciduous temperate shrub |
| 11 | Broadleaf deciduous boreal shrub |
| 12 | Cool/Arctic C3 grass |
| 13 | C3 grass (cool) |
| 14 | C4 grass (warm) |
| 15 | Crop 1 (Corn) |
| 16 | Crop 2 (Other crops) |
| 17 | Barren land |

20.6 Leaf area index

The leaf area index (LAI) in Oslo CTM3 is actually green leaf area index, but we still call it LAI. It is taken from

Table 26: MODIS-PFTs.

| # | Name |
|----|------------------------------------|
| 1 | Evergreen Needleleaf Forests |
| 2 | Evergreen Broadleaf Forests |
| 3 | Deciduous Needleleaf Forests |
| 4 | Deciduous Broadleaf Forests |
| 5 | Mixed Forests |
| 6 | Closed Shrublands |
| 7 | Open Shrublands |
| 8 | Woody Savannas |
| 9 | Savannas |
| 10 | Grasslands |
| 11 | Permanent Wetlands |
| 12 | Croplands |
| 13 | Urban and Built-Up |
| 14 | Cropland/Natural Vegetation Mosaic |
| 15 | Permanent Snow and Ice |
| 16 | Barren or Sparsely Vegetated |
| 17 | Unclassified |

ISLSCP2, FASIR adjusted, in 0.25 degree resolution, (Sietse et al., 2010). The field is interpolated to Oslo CTM3 resolution.

The path to the file is set in the input file, along with the year to apply, `LAI_YEAR`. Only year 1982 to 1998 are available, so for general model studies we use the climatological mean of these, set by `LAI_YEAR=0000`. If you set 9999, the meteorological year will be used (if available).

20.7 Roughness length

The roughness length (`ZOI`) is taken from ISLSCP2, FASIR adjusted, in 0.25 degree resolution, (Sietse et al., 2010). The field is interpolated to Oslo CTM3 resolution.

The path to the file is set in the input file, along with the year to apply, `ZOI_YEAR`. Only year 1982 to 1998 are available, so for general model studies we use the climatological mean of these, set by `LAI_YEAR=0000`. If you set 9999, the meteorological year will be used (if available).

21 Diagnostics

In the Oslo CTM3 we try to do all processes in parallel regions (private arrays), and this also applies for the diagnostics. This is done either by creating private arrays for diagnostics, which are then put back to global arrays at the end of the parallel region, or by letting the parallel region work directly on its part of a global array – in that case the global array should be set up for IJ-block structure (see Section 4.3.2 for more on that).

21.1 Core diagnostics

The simplest diagnostics is the 3D averages, but the core can also diagnose each process.

The process diagnostics can be calculated in 2D (zonal

means or layers), for pre-defined boxes, and in addition time series can be produced. The core diagnostics are controlled by flags in the input file *LxxCTM.inp*.

21.1.1 3D averagees

Averages of all species are calculated. The 3D average in the Oslo CTM2 was monthly averages. In the Oslo CTM3, however, you are more free to set the temporal span of the average.

In the file *LxxCTM.inp* you can set flags for when to calculate averages (AVERAGES calendar `JD0_A`). The shortest time span is one day, and the time span is the period since the last average calculation. Setting the flags to 1 generates the files, while setting it higher than 1 also prints some data to screen.

Since mid-2017, The file format for averages is netCDF4, and the file name is *avgsavFROMDATE_TODATE.nc*, where `FROMDATE` and `TODATE` are on the form `YYYYMMDD`. Hourwise, the accumulation starts at 00UTC on `FROMDATE`, and runs until 00UTC on `TODATE` (00UTC on `TODATE` is thus taken into account in the next average).

Note that the program will stop if the *avgsav*-file already exist. This is to prevent results from being overwritten.

The plan is that only selected species (listed in input file) will be written to 3D averages, to save space.

All variables put to file are described in the file, and they are:

The variable dimensions on file:

- `lat`: Latitudinal dimension
- `lon`: Longitudinal dimension
- `lev`: Vertical dimension
- `ilat`: `lat+1`
- `ilon`: `lon+1`
- `ilev`: `lev+1`
- `tname_len`: Length of character strings in `TNAME`
- `date_size`: 6 (year, month, date, hour, minutes, seconds)

The fixed (not average) variables are:

- `lon`: Longitudes at grid box center. Unit is degrees East.
- `lat`: Latitudes at grid box center. Unit is degrees North.
- `lev`: Pressure at mass-weighted grid box center (mean of pressures at upper and lower edges), assuming surface at 1000hPa. Unit is hPa.
- `ilon`: Longitude at at eastern edges of grid boxes. Unit is degrees East.
- `ilat`: Latitudes at southern edges of grid boxes. Unit is degrees North.
- `ilev`: Pressure at lower edge of grid box, assuming surface at 1000hPa. Unit is hPa.
- `ihya`: Sigma hybrid coordinate A, called **ETAA** in Oslo CTM3. Unit is hPa.
- `ihyb`: Sigma hybrid coordinate B, called **ETAB** in Oslo CTM3. Unitless.
- `IPARW`: Meteorological data native longitudinal resolution.

- JPARW: Meteorological data native latitudinal resolution.
- LPARW: Meteorological data vertical resolution.
- NRAVG: Number of time steps accumulated.
- START_TIME: Start time [YYYY,MM,DD,hh,mm,ss] for accumulating data.
- END_TIME: End time [YYYY,MM,DD,hh,mm,ss] for accumulating data.
- START_DAY: Start day for accumulating data (model counter NDAY).
- END_DAY: End day for accumulating data (model counter NDAY).
- VERSION: Output file version number.
- NPAR: Number of transported species in simulation.
- NOTRPAR: Number of non-transported species in simulation.
- tracer_idx: ID numbers for species used in Oslo CTM3(chem_idx and Xchem_idx).
- tracer_molweight: Molecular weight for transported species. Unit is g/mol.
- tracer_name: Tracer/species names.
- tracer_transported: Flag if tracer was transported (1) or not (0).
- gridarea: Grid box area. Unit is m².

The averaged variables are:

- Psfc: Surface pressure. Unit is hPa.
- AIR: Grid box air masses. Unit is kg.
- volume: Grid box air volumes. Unit is m³.
- air_density: Grid box air density. Unit is molec/cm³.
- temperature: Grid box temperature. Unit is K.
- height: Height of grid box bottom, so it is of size LPAR+1, and it has reverse order (ilev,lon,lat).
- LMTROP: Uppermost model level in troposphere.
- H2O_all: H₂O from metdata Q, but overwritten in the stratosphere by calculated H₂O when available.
- Q: Specific humidity retrieved from meteorological data. Unit is kg(H₂O)/kg(air).
- Tracers: All included tracers. Units are kg of species.

21.1.2 Process diagnostics / budget diagnostics

All processes are diagnosed. However, when the Oslo treatment of emissions and deposition is used, those processes will not be diagnosed well, as they are part of the chemistry. However, they are diagnosed separately.

Budget diagnostics of different processes are controlled by the BUDGET tendencies calendar (JDO_T) in the input file.

21.1.3 e90 tracer

Prather et al. (2011) presented a tracer that with given surface emissions and an e-folding atmospheric lifetime of 90 days, will follow the observed tropopause closely at about 90 ppbv.

This is used to set the 3D logical variable LSTRATAIR_E90, where .true. is stratospheric air. It uses a specific volume mixing ratio for the E90 tracer, given by E90VMR_TP (Prather et al., 2011).

You can turn this tracer on in *Makefile*.

The e90 tracer is so far used for flux calculations (Section 21.1.4), but could in the future also be used for selecting tropospheric or stratospheric chemistry scheme, either as a 3D field or by selecting the uppermost tropospheric grid box as tropopause, similar to the PVU-based tropopause. Note that the program code is not set up for a 3D definition.

21.1.4 Stratosphere-Troposphere-Exchange

In Oslo CTM3 the stratosphere-troposphere-exchange (STE) calculation follows Hsu et al. (2005), and requires that the e90 tracer is included (Section 21.1.3). STE is calculated based on the calculated O₃, with the possibility to also calculate STE for a Linoz O₃ tracer.

During a certain time period in Oslo CTM3 (e.g. a month), STE of O₃ is calculated as a residual of column mass budgets between the model surface and a certain O₃ isopleth (Hsu et al., 2005). Below the given isopleth and for the given time period, this can be written

$$\left(\frac{dM}{dt}\right)_{tot} = \left(\frac{dM}{dt}\right)_{chem} - S + F_{s \rightarrow t} - F_{h,t \rightarrow t} \quad (143)$$

where $\left(\frac{dM}{dt}\right)_{tot}$ is the total change in O₃, $\left(\frac{dM}{dt}\right)_{chem}$ is the corresponding chemical tendency of O₃ and S is sink processes such as dry deposition at the surface and wet scavenging. $F_{s \rightarrow t}$ is the STE to be inferred (both horizontal and vertical), and $F_{h,t \rightarrow t}$ is the horizontal flux of O₃ from tropospheric air to tropospheric air (positive out of the column). The latter is found by comparing the volume mixing ratio of the flux to the isopleth values, and account for values lower than the isopleth (i.e. the partly tropospheric air in a gridbox). The calculation of $F_{h,t \rightarrow t}$ is explained at the end of this Section.

For post-processing, it is also worth noting that $F_{h,t \rightarrow t}$ and $\left(\frac{dM}{dt}\right)_{tot}$ may need to be filtered to reduce noisy plots – see the end of this Section for more on that.

Back to Eq (143), the left-hand side is thus diagnosed as the change from the beginning to the end of the time period, while the right-hand side terms (except $F_{s \rightarrow t}$) are summed up for all time steps during the time period.

Note that this is the same treatment as used by Stevenson et al. (2006); but instead of separating the P and L terms for tropospheric O₃ (which is somewhat arbitrary and often based on a concept of odd-oxygen) we diagnose the sum $P-L$ as $(dM/dt)_{chem}$ in Eq (143) and the deposition D as S . Assuming no tropospheric trend, as in Stevenson et al. (2006), means that $(dM/dt)_{tot} + F_{t \rightarrow t} = 0$ in our equation.

The use of the 120 ppb O₃ surface for calculating STE may be problematic in very polluted regions, e.g. in biomass burning areas. This has been solved by forcing the diagnose to assume all air below 4 km altitude to be tropospheric, and between 30 S and 30 N air is assumed to be tropospheric all the way to the tropopause.

Similarly, the use of 150 ppb may confuse stratospheric O₃-hole air with tropospheric air if O₃ is below 150 ppb.

A better diagnose is probably to use a surface independent of O₃, such as the e90-stratosphere definition, as basis for Eq (143). This is included in the CTM3, found to produce approximately similar STE as the 120 ppb O₃ surface (Søvde et al., 2012). Also for this diagnose air below 4 km is assumed tropospheric.

An additional possibility is to use Linoz O₃ tracer for STE calculations. The Linoz tracer is turned on with a separate option in *Makefile*, and this tracer needs to be called 03LINOZ. It should be noted that CTM3 is not set up to use Linoz instead of the stratospheric chemistry module, only as an STE diagnostic. See Section 11.7 for more.

How often STE is to be diagnosed, is set in the input file, by the flags in JD0_X calendar. The whole STE budget is written to file *ste_YYYYMMDD_YYYYMMDD.nc*, where the first date is the start time (00UTC) of STE calculation and the latter date is the end of the calculation (also at 00UTC).

To summarize, STE can be calculated when stratospheric O₃ is present, either through CTM3 stratospheric chemistry or by Linoz. Also, you have to include the e90 tracer in the *Makefile* settings.

Calculation of $F_{h,t \rightarrow t}$ using e90-tracer

This is also explained in detail in the source code (*ste_flux.f90*). This flux is called QFU and QFV in Oslo CTM3, and in the source code you find them in *ste_flux.f90* and also in *p-vect3.f*. These variables give the tracer mass transported from one grid box to the next, and also the first moments For *U* these are QFU(:, :, 1) and QFU(:, :, 2), respectively. Similarly, QFV(:, :, 1) and QFV(:, :, 2), are for *V*.

In the STE diagnose, we need to keep track of the flux from tropospheric to tropospheric grid boxes, i.e. $F_{h,t \rightarrow t}$. To decide whether the air is tropospheric, stratospheric or both, we apply the mean flux of the e90 tracer out of the grid box (Q0F_E90) and the first moment (Q1F_E90). Figuratively, Q0F_E90 and Q1F_E90 set up a trapezoid, with left top point at

$$h_L = |Q_{0F,E90}| + |Q_{1F,E90}| \quad (144)$$

and right top point at

$$h_R = |Q_{0F,E90}| - |Q_{1F,E90}| \quad (145)$$

The signs in front of the moments are opposite of the original CHEMFLUX routine, where the O₃ gradient is used: e90 and O₃ has opposite gradients.

Stratospheric air is found when the mass mixing ratio of the e90-tracer is smaller than the tropopause value, called F_0 in the routine, and we do this comparison for the mass mixing ratio in the flux:

Tropospheric air

Mass in left corner of trapezoid is higher than the stratospheric limit $F_0 * \text{abs}(QU)$, where QU is air flux:

$$F_0|QU| < |Q_{0F,E90}| - |Q_{1F,E90}| \quad (146)$$

Stratospheric air

Mass in right corner of trapezoid is lower than the strato-

spheric limit:

$$F_0|QU| \geq |Q_{0F,E90}| + |Q_{1F,E90}| \quad (147)$$

Partly tropospheric and partly stratospheric air

We need to locate the tropopause first. Having the range of the trapezoid x-axis [0,1], the tropopause lies within, at a point X . X is therefore the fraction of tropospheric air, and lies between h_L in Eq. (144) and h_R in Eq. (145):

$$|Q_{0F,E90}| + |Q_{1F,E90}| - 2X|Q_{1F,E90}| = F_0|QU| \quad (148)$$

Rearranging:

$$X = -\frac{F_0|QU| - |Q_{0F,E90}| - |Q_{1F,E90}|}{2|Q_{1F,E90}|} \quad (149)$$

The stratospheric fraction is therefore (perhaps more easily) derived by looking from right to left on the trapezoid:

$$X_f = (1 - X) = \frac{F_0|QU| - |Q_{0F,E90}| + |Q_{1F,E90}|}{2|Q_{1F,E90}|} \quad (150)$$

To avoid dividing by zero, we limit the divisor ($|Q_{1F,E90}|$) by $10^{-10}|Q_{0F,E90}|$.

Again: Note that when using $|Q_{0F}|$ and $|Q_{1F}|$ for O₃ to calculate the tropospheric fraction, X_f is effectively the *tropospheric* fraction because its gradient is opposite of E90.

Having the stratospheric fraction X_f , and the tropospheric fraction $X = (1 - X_f)$, we calculate the O₃ flux at X , which we call Y .

$$Y = |Q_{0F,O3}| - |Q_{1F,O3}| + (1 - X_f)2|Q_{1F,O3}| \quad (151)$$

The basis for this equation is that the O₃ gradient and E90 gradient have opposite signs, so we interpolate the O₃ flux linearly from the left corner of the O₃ trapezoid (tropospheric part), to the tropopause value at X .

Having the flux ($|Q_{0F,O3}| - |Q_{1F,O3}|$) at the left corner of the O₃ trapezoid and Y at the point $(1 - X_f)$, we integrate over the trapezoid, i.e. finding the area bound by $x = [0, 1 - X_f]$ and $y = [|Q_{0F,O3}| - |Q_{1F,O3}|, Y]$ to find the tropospheric part of the flux:

$$F_{h,t \rightarrow t} = (|Q_{0F,O3}| - |Q_{1F,O3}| + Y)(1 - X_f)/2 \quad (152)$$

Why integrate? While $Q_{0F,O3}$ is the mean flux out of the box, we use the moments and find the flux (i.e the grid box mass transported to the neighbor box) at both ends of the trapezoid. The total mass transported equals the area of the trapezoid.

Filters

The calculation of STE may result in a noisy figure when plotted as a map. To reduce the noise, UCI uses a 1-2-1 filter (0.25:0.5:0.25 weights) for $F_{h,t \rightarrow t}$ and for $\left(\frac{dM_t}{dt}\right)_{tot}$, given in Table 27.

I am not totally confident in this method, but in any case, it should be done in post-processing data, not for calculating the global STE in Oslo CTM3. Hence, this is not included in the netCDF output file.

Table 27: UCI filter method for $F_{h,t \rightarrow t}$ and $(\frac{dM_t}{dt})_{tot}$ when calculating STE.

```

!// For hflx, do 1-2-1 filtering twice:
do k = 1, 2
  do j = 1, jpar
    do i = 1, ipar
      ib = mod(i, ipar) + 1
      ia = mod(i-2+ipar, ipar) + 1
      hflx(i,j) = 0.25 * hflx(ib,j)
                + 0.50 * hflx(i,j)
                + 0.25 * hflx(ia,j)
    end do
  end do
  !// Skip polar-most boxes:
  do j = 6, jpar - 5
    do i = 1, ipar
      hflx(i,j) = 0.25 * hflx(i,j-1)
                + 0.50 * hflx(i,j)
                + 0.25 * hflx(i,j+1)
    end do
  end do
end do

!// For dm, do 1-2-1 filtering once:
do j = 1, jpar
  do i = 1, ipar
    ib = mod(i, ipar) + 1
    ia = mod(i-2+ipar, ipar) + 1
    dm(i,j) = 0.25 * dm(ia,j)
             + 0.50 * dm(i,j)
             + 0.25 * dm(ib,j)
  end do
end do
!// Do all but polar boxes first:
do j = 2, jpar-1
  do i = 1, ipar
    dm(i,j) = 0.25 * dm(i,j-1)
             + 0.50 * dm(i,j)
             + 0.25 * dm(i,j+1)
  end do
end do
!// Override polar boxes:
do i = 1, ipar
  dm(i,jpar) = dm(i,jpar-1)
  dm(i,1) = dm(i,2)
end do

```

21.2 Oslo CTM3 diagnostics

There are several diagnostics developed for the Oslo CTM2 that are inherited by the Oslo CTM3. The diagnoses are generally located in the files *diagnostics_general.f90*. However, there are also some scavenging diagnostics given in *diagnostics_scavenging.f90*.

21.2.1 Chemical production and loss

Production and loss terms for selected species are accumulated during chemistry routines. Only some species are included in this diagnose so far, namely CH₄, N₂O and a few others. The routine doing the summing is `save_PL`.

If you need to include more diagnostics, look for `CHEMLOSS` and `CHEMPROD` in the chemistry routines.

These budget terms, along with the tracer burdens, can be put out in the routine `chembud_output`.

Note that some species are difficult to diagnose, such as O₃, which is calculated by the use of the O_x family concept.

The diagnosed losses are used to calculate lifetimes, as will be described in Section 21.2.2.

21.2.2 CH₄ and N₂O burdens and lifetimes

When running the Oslo CTM3 with full chemistry, the burdens and lifetimes of N₂O and CH₄ are calculated out. The diagnoses can be found in *diagnostics_general.f90*.

Average burden of N₂O and CH₄ are diagnosed in `ch4n2o_burden`, while chemical loss is summed up in `ch4_loss3` and `n2o_loss3`.

Calculations are done between the surface and

- the model tropopause level.
- 200 hPa.
- the 150 ppbv O₃ surface.
- the model top.

Instant, monthly means and running monthly means are printed to standard out. This is done in the routine `report_ch4n2o`, called from `REPORTS_CHEMISTRY`.

Note that while CH₄ is lost only to OH in the troposphere, it is also lost to O(¹D) and Cl in the stratosphere, reducing the lifetime compared to a pure OH diagnostic. See also Section 21.2.3 for atmospheric OH and additional CH₄ lifetime calculations.

Also note that even though all the loss terms may be diagnosed from chemistry, the lifetime concept may not hold if there are large sources. If you include CH₄ emissions, the method may not give the correct lifetime. However, we assume minimal impact on the loss and hence report the calculated lifetime anyway.

21.2.3 OH and CH₄ lifetimes

The routine `sumup_burden_and_lifetimes` calculates atmospheric OH in different ways:

- OH-average CH₄-kernel, Eq. (153), from surface to model top.
- OH-average CH₄-kernel from surface to LMTR0P (not printed by default).
- OH-average CH₄-kernel from surface to 200 hPa (not printed by default).
- OH-average CO-kernel, Eq. (154), from surface to model top.
- Spivakovsky et al. (2000)
- Lawrence et al. (2001)

Summing up throughout the domains listed above.

CH₄ kernel:

$$\overline{\text{OH}}_{\text{CH}_4} = \frac{\sum m_a k_{\text{OH}+\text{CH}_4} [\text{OH}]}{\sum m_a k_{\text{OH}+\text{CH}_4}} \quad (153)$$

where m_a is air mass (kg), and $[\text{OH}]$ is concentration (molecules/cm³) and $k_{\text{OH}+\text{CH}_4}$ is the reaction rate for $\text{OH} + \text{CH}_4$.

CO kernel:

$$\overline{\text{OH}_{\text{CO}}} = \frac{\sum m_a k_{\text{OH}+\text{CO}} [\text{OH}]}{\sum m_a k_{\text{OH}+\text{CO}}} \quad (154)$$

Instantaneous and running averages are reported by `report_burden_and_lifetime`, which is called from `REPORTS_CHEMISTRY`.

Lifetimes using the CH_4 kernel and the Lawrence method are printed to standard out.

21.2.4 Atmospheric burdens

The routine `diag_burden_snapshot`, called from `REPORTS_CHEMISTRY`, puts out instantaneous tropospheric and stratospheric burdens of selected species. This is done for each meteorological time step, and currently only O_3 . Other species can be included easily.

Generally it is not very useful to print instantaneous burden that often, so I have restricted it to O_3 so far.

21.2.5 Atmospheric lifetimes

It is possible to add calculation of other chemical lifetimes; if you want to do that, you should follow the method for CH_4 and N_2O .

Note also that aerosol packages generally have their own calculations of lifetimes.

21.2.6 Time series of vertical profiles

Time series of vertical profiles, for given stations, are included. The code can be found in the file `verticalprofiles_stations2.f90` in the `OSLO` directory. Species are diagnosed at the beginning of each NOPS (i.e. for every hour in standard settings), for each station grid box.

Using the station location (latitude and longitude), this routine linearly interpolates horizontally from the 4 closest grid boxes.

An IDL program for reading this output is available in the SVN repository (see Section B).

You specify species to diagnose in the file `verticalprofiles_stations2.f90`. Some meteorological components are also diagnosed, e.g. temperature, pressure, model grid height, air mass, equivalent latitude, etc.

As input the program reads a file `station-list_verticalprofiles.dat` at model start, while output is done at the beginning of each day (i.e. after start day), in the file `hourly_station_vprof_YYYYMMDD.dta`. The stations used in the standard output are shown in Figure 2.

List of output data for each daily file:

- **year:** Year.

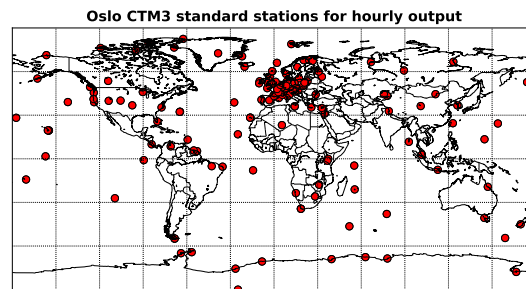


Figure 2: Map of stations included in the standard output for vertical profiles.

- **month:** Month of year.
- **date:** Date of month.
- **LPAR:** Number of vertical layers.
- **ntracer:** Number of tracers diagnosed.
- **nrofstations:** Number of stations.
- **NTHE:** Number of θ -levels for equivalent latitude.
- **actual_diag:** Number of NOPS steps diagnosed, i.e. $\text{NROPSM} * \text{NRMETD}$.
- **etaa:** Sigma coordinate A (η_a) for all levels.
- **etab:** Sigma coordinate B (η_b) for all levels.
- **stt_components:** Tracer ID numbers diagnosed.
- **mole_mass:** Molecular mass of tracers.
- **pvthe:** Theta levels for equivalent latitude.

List of output data for each station:

- **locname:** Station name.
- **loccode:** Station 3-char code.
- **lat:** Latitude.
- **lon:** Longitude.
- **alt:** Altitude.
- **ii:** CTM zonal grid box index.
- **jj:** CTM meridional grid box index.
- **nb_ii:** Zonal neighbor grid box index.
- **nb_jj:** Meridional neighbor grid box index.
- **nb_xfrac:** Fractional distance to zonal neighbor.
- **nb_yfrac:** Fractional distance to meridional neighbor.
- **areaxy:** Grid box area [m²] (interpolated).

For all diagnostic steps, the following data are stored:

- **psfc:** Surface pressure [hPa].
- **BLH:** Boundary layer height [m].
- **mass:** Tracer masses [kg/grid box].
- **h2o:** H_2O mass [kg/grid box].
- **temperature:** Temperature [K].
- **airmass:** Air mass [kg/grid box].
- **zoflev:** Height of grid box bottoms [m].
- **eqlat:** Equivalent latitude on theta levels.
- **PVU:** Potential vorticity units.
- **tph_pres:** Tropopause pressure [hPa].

21.2.7 Satellite vertical profiles

A routine for putting out vertical profiles at given locations and times, e.g. satellite positions, are included in the file `satelliteprofiles_mls.f90`. In this file you define which tracers to put out. Some meteorological components are also diagnosed, e.g. temperature, pressure, model grid

height, air mass, equivalent latitude, etc. Using the satellite profile location (latitude and longitude), this routine linearly interpolates horizontally from the 4 closest grid boxes. In the future, it may be better to save data for all columns and do interpolation in post-processing. Due to the large amount of data per file, this is not done now.

Since each profile is taken between some start time of NOPS and start time of NOPS+1, output is given for both NOPS and NOPS+1, allowing temporal interpolation as well.

List of output data for each daily file:

- **year:** Year.
- **month:** Month of year.
- **date:** Date of month.
- **LPAR:** Number of vertical layers.
- **ntracer:** Number of tracers diagnosed.
- **nsatprofs:** Number of profiles.
- **NTHE:** Number of θ -levels for equivalent latitude.
- **etaa:** Sigma coordinate A (η_a).
- **etab:** Sigma coordinate B (η_b).
- **stt_components:** Tracer ID numbers diagnosed.
- **mole_mass:** Molecular mass of tracers.
- **pvthe:** Theta levels for equivalent latitude.

List of output data for each profile:

- **time:** Time of observation.
- **time_sec:** CTM NOPS times before and after.
- **lat:** Latitude.
- **lon:** Longitude.
- **ii:** CTM zonal grid box index.
- **jj:** CTM meridional grid box index.
- **nb_ii:** Zonal neighbor grid box index.
- **nb_jj:** Meridional neighbor grid box index.
- **nb_xfrac:** Fractional distance to zonal neighbor.
- **nb_yfrac:** Fractional distance to meridional neighbor.
- **areaxy:** Grid box area [m²] (interpolated).

For the two closest NOPS steps, the following data are stored:

- **psfc:** Surface pressure [hPa].
- **BLH:** Boundary layer height [m].
- **mass:** Tracer masses [kg/grid box].
- **H2O:** H₂O mass [kg/grid box].
- **temperature:** Temperature [K].
- **airmass:** Air mass [kg/grid box].
- **zoflev:** Height of grid box bottoms [m].
- **eqlat:** Equivalent latitude on theta levels.
- **PVU:** Potential vorticity units.
- **tph_pres:** Tropopause pressure.

21.2.8 O₃ column

Tropospheric and total columns of O₃ are diagnosed in the subroutine *du_columns* in the file *diagnostics_general.f90*. It is called from *mp_diag*, which does diagnoses in each IJ-block.

The columns are diagnosed every meteorological time step (NMET) and are stored once every day. This is carried out in the routine *write_ducolumns*.

21.2.9 3-hourly output

Oslo CTM3 has the possibility of putting out 3-hourly instantaneous fields, mostly O₃ and aerosols. These are e.g. used for RF calculations.

You turn this diagnose on by setting `LDUMP3HRS=.true.` at the top of the file *gmdump3hrs.f90*, and the main routine is *dump3hrs*.

If you want to add other components than O₃, this is of course possible. When you understand the code, it should be easy to implement.

21.2.10 Snapshots on θ -levels

In the routine *write_snapshot_the*, located in *diagnostics_general.f90*, you can put out instantaneous mixing ratios of selected species, interpolated to the potential temperature (θ) levels defined in the physics routine, see Section 20.3. The number of θ -levels (*pvthe*) are given by *NTHE*.

Routine puts out data every hour, and the default species put out are O₃ and N₂O, along with PVU and equivalent latitude.

Routine can put out data for only one hemisphere or both. See the source code for how to change it.

The routine is called from *nops_diag*, but is commented out by default. A second routine, *write_snapshot*, is also available, putting out gridbox mass of selected species on model levels.

21.2.11 Emission tendencies

When emissions are treated as production terms in chemistry, i.e. in standard Oslo chemistry, the total emitted per day is calculated for all species, in *tnd_emis_daily*. This is explained in Section 8.10.

A Description of model files

Here the source files are described. Generally, files inherited from UCI are placed in the main directory, while the OSLO chemistry and physics are placed in the directory *OSLO*. The files in the main directory is often referred to as the core files, and will be described next.

A.1 UCI core source files

The Oslo CTM3 started out based on the UCI CTM version 5.6d, but was later updated to 6.1b, before most of the UCI code was restructured into Fortran90 free format, and all common blocks were abandoned. In this process I renamed most of the files. Future core update should be fairly straight-forward for a somewhat experienced user.

This Section describes the core files necessary to run the Oslo CTM3. If you want to go back and see the UCI

codes, you should contact UCI.

First the global variable files (common files) are listed, then the core files are listed alphabetically.

A.1.1 *cmn_precision.f90*

This file defines the precision of the Oslo CTM3 floating point variables. Several are used:

- r8 Double precision. Most variables use this.
- r4 Single precision.

rMom Precision of the second order moments. By default this is single precision.

rAvg Precision of the global average arrays. By default this is single precision.

rTnd Precision of the global tendency arrays. By default this is single precision.

A.1.2 *cmn_size.F90*

Contains the array size parameters and flags. Examples are IPAR, IPARW, JPAR, JPARW, LPAR, LPARW, MPIPAR, MPJPAR, NRMETD, NPAR, etc.

A.1.3 *cmn_parameters.f90*

Contains chemical and physical parameters, such as the Earth radius (A0), Avogadro's number (AVOGRN), Apparent molecular weight of dry air (M_AIR), gas constants (R_AIR, R_UNIV, R_ATM), and many more. These are all listed in Table 28.

A.1.4 *cmn_ctm.f90*

Defines the main arrays for the transport model, such as STT and the moments (SUT, SVT, SWT, SUU, SVV, SWW, SUV, SUW, SVW).

Also grid info such as longitude (XGRD, XDGRD, XEDG, XDEDG), latitude (YGRD, YDGRD, YEDG, YDEDG), and sigma hybrid coordinates (ETAA, ETAAW, ETAB, ETABW) are defined here.

A.1.5 *cmn_chem.f90*

Defines the main arrays for emissions and chemistry, such as E3DSNEW (LPAR, IPAR, JPAR, E3PAR) and the tables mapping species to emission datasets:

- NE2TBL: Total number of 2D emission datasets.
- NM2TBL: Table of months the emissions apply for.
- NY2TBL: Table of months the emissions apply for.
- E2DS: All 2D emission datasets.
- E2LTBL: Table mapping species to 2D emission datasets.
- E2STBL: Table of scaling factors for the mapping of each species and 2D emission datasets.

Similar arrays exist for 3D emissions.

Here you also find the tracer name TNAME, tracer molecular weight TMASS, and other variables such as conversion factors TMASSMIX2MOLMIX and TMOLMIX2MASSMIX.

The variables are generally well described in the source code.

A.1.6 *cmn_diag.f90*

Defines arrays for diagnostics, such as STTAVG, AIRAVG, JDO_A.

A.1.7 *cmn_fjx.f90*

Defines fast-JX parameters and arrays.

A.1.8 *cmn_met.f90*

Defines meteorological arrays.

A.1.9 *cmn_sfc.f90*

Defines surface variables such as land surface type (landSurfTypeFrac), land-sea mask (LSMASK), and dry deposition velocity (VDEP).

A.1.10 *averages.f90*

Contains routines for summing up 3D averages.

- AVG_WRT_NC4: Write core 3D averages (the avgsav-files), including XSTT averages, surface pressure averages (which is 2D), and some meteorological averages.
- AVG_ADD2: Add to 3D averages.
- AVG_CLR2: Clear 3D averages.
- AVG_P1: Write 1D averages to screen.
- AVG_WRT2: Only included for history. See AVG_WRT_NC4. Write core 3D averages (the avgsav-files), including XSTT averages, surface pressure averages (which is 2D), and several meteorological averages.

A.1.11 *budgets.f90*

Contains routines for summing up tendency budgets.

- TBGT_G: Clear budget arrays.
- TBGT_L: Accumulate budgets layerwise.
- TBGT_IJ: Accumulate budgets in IJ-block.
- TBGT_P0: 0D print to screen.
- TBGT_P1: 1D print to screen.
- TBGT_P2: 2D print to screen.

A.1.12 *cloudjx.f90*

Routines for treating cloud-J. Currently set up for cloud2 as used by fast-JX 6.7c, but will be updated when fast-JX 7.3c is included.

- cloud_init: Initialise cloud-J.

Table 28: Parameters defined in *cmn_parameters.f90*.

| Name | Value | Description |
|-----------|--------------------------|---|
| AO | 6371000 | Earth radius [m] |
| GO | 9.80665 | Gravitational constant [m/s ²] |
| CPI | 3.141592653589793 | π |
| C2PI | 2*CPI | 2π |
| CPI180 | CPI/180 | Conversions to radians |
| ZPI180 | 1/CPI180 | Conversions from radians |
| atm2Pa | 101325 | Conversion from atmospheres to Pa |
| Pa2atm | 1/atm2Pa | Conversion from Pa to atm |
| J2kcal | 4186.8 | Numbers of kcal in a J |
| M_AIR | 28.97 | Molecular mass for air [g/mol] |
| R_UNIV | 8.31446 | Universal gas constant [J/(K mol)] = [m ³ *Pa/(K mol)] |
| R_ATM | R_UNIV * Pa2atm | Gas constant in [m ³ *atm/(K mol)] ($\sim 8.205d-5$) |
| R_AIR | R_UNIV / M_AIR * 1000 | Specific gas constant for air [J/(K kg)] (~ 287) |
| R_H2O | R_UNIV / 18.01528 * 1000 | Specific gas constant for water vapor [J/(K kg)] (~ 461) |
| AVOGRN | 6.022149e23 | Avogadro's number [molecules/mol] |
| BOLTZMANN | 1.38063e-23_r8 | Boltzmann's const [J/(K molecules)] |
| KBOLTZ | 1.e4_r8 * BOLTZMANN | Boltzmann's const [mb cm ³ /(K molecules)] |
| cp_air | 1004 | Specific heat of dry air at constant pressure [J/(K kg)] |
| Lv_OC | 2.501e6_r8 | Latent heat of vaporization at 0°C [J/kg] |
| dLv_dT | -0.00237e6_r8 | Gradient of Lv between 0C and 100C [(J/kg)/K] (Table C-5 in Stull, 1988) |
| TK_OC | 273.15 | Temperature [K] at 0°C |
| es_OC | 611.2 | Saturation vapor pressure of H ₂ O at 0°C [Pa] |
| secDay | 86400 | Seconds in a day |
| secYear | 31536000 | Seconds in a year |
| MINTEMP | 150 | Minimum temperature allowed in chemistry |
| MAXTEMP | 350 | Maximum temperature allowed in chemistry |
| TEMPRANGE | MAXTEMP - MINTEMP | Temperature range. |
| LDEBUG | .true. | Global flag for including more extensive debugging. |

- RANSET: Set random number. Random seed is **A.1.14** *fastjx.f90*
RANSEED, which is set in *LxxCTM.inp*.

Some important variables for cloud2:

- LCLDAVG:
- LCLDQMD:
- LCLDQMN:
- LCLDRANA:
- LCLDRANA:

A.1.13 *convection.f90*

This is the f90 version of the UCI *p-cnvw.f*. It has been modified to Oslo CTM3, calculating elevator fractions, and also the Henry coefficients used in convective washout. A new convective wet loss variable is included; CNV_WETL (LPAR,NPAR).

- CONVW_OSL0: The main routine.
- ADJFLX2: Adjust convective fluxes so that no more than a fraction of the grid box mass is moved each time step.
- ADJFLX Old version of ADJFLX2.
- QCNVW2_OSL0: Column model calculating convective transport, and also convective scavenging by up-drafts.
- QCNVW2: UCI routine kept for history.
- SCAV_UPD: UCI routine kept for history.

Contains routines for fastJX, except the main driver which is so far located in *p-phot_oc.f*. That will change when fast-JX is updated to 7.3.

- RD_XXX: Reads *FJX_spec.dat*.
- RD_MIE: Reads *FJX_scat.dat*.
- RD_JS: Reads *ratj_oc.d* file.
- RD_01D: Reads 01D entry of *ratj_oc.d* file.
- SET_ATM: Reads O₃ and temperature climatologies to use above the model domain. It can possibly be used in the stratosphere when stratospheric chemistry is not included, but Oslo CTM3 uses its own climatology for that. Sets e.g. TOPT, TOPM, TOP3.

Changes compared to UCI p-phot.f file

In the subroutine PHOT_IN a small piece of ASAD code was removed. Some other ASAD variables has been removed.

Also, the subroutine SET_ATM had to be modified to include climatology data for the uppermost layer (LPAR3, LPART and LPARM).

A.1.15 *grid.f90*

Routines for setting up model grid.

- SET_GRID: Sets up global grid, such as latitude, longitude, area of grid boxes, etc.

- LABELG: For printing grid info to screen.
- DIAGBLK: Finds grid box start/end indices for box diagnose.
- DIAG_LTSTN: Finds grid box indices for station diagnose.
- DIAG_LTGL: Finds grid box indices for local time station diagnose.
- GAUSST2: Calculate Gaussian quadrature points and weights.
- DBLDBL: Define longitude and latitude of horizontally degraded grid.
- AIRSET: Sets up 3D air mass.
- SURF_IN: Reads land fraction datasets.
- gridICAO: Not used. I think this finds grid for some ICAO emission data.

A.1.16 *initialize.f90*

Routines for initializing the Oslo CTM3.

- INPUT: Reads *LxxCTM.inp*.
- SETUP_SPECIES: Reads restart file.
- SETUP_UNF_OUTPUT: Opens unformatted output files (UCI heritage).
- report_zeroinit: Reports which tracers are initialized to zero (i.e. not read from file).

A.1.17 *lightning.f90*

Contains routines for calculating lightning NO_x (L-NO_x) emissions. There are several methods for doing this, as described in Section 8.8.

- getScaleFactors: Sets scaling factors based on which meteorological dataset is used.
- LIGHTNING_OAS2015: Default method for calculating L-NO_x.
- LIGHTNING_GMD2012: L-NO_x as described by Søvde et al. (2012).
- LIGHTNING_UCI2015: L-NO_x as used by UCI-CTM in 2015. I do not recommend using this.
- LIGHTDIST: Sets up vertical distribution of L-NO_x.
- filterLNC: Filter convective mass fluxes to reduce noise in L-NO_x horizontal distribution.
- distland: Finds grid boxes that are land or have land in 300 km proximity. Test routine to make land near-land lightning behaving like land. **Not used.**
- LIGHTNING_ALLEN2002: L-NO_x as described by Allen and Pickering (2002). Not evaluated.

A.1.18 *metdata_ecmwf.f90*

Read-in for ECMWF IFS meteorological data on netCDF4 format.

- update_metdata: Updates meteorological data.
- fluxfilter2: Filter convective mass fluxes; removes noise.
- data2mpblocks: Puts globally gridded (IPAR, JPAR) data into IJ-block (IDBLK, JDBLK, MPBLK).
- gotData: Prints info to standard out.
- skipData: Prints info to standard out.

A.1.19 *metdata_ecmwf_uioformat.f90*

Traditional read-in for ECMWF IFS meteorological data on UIO binary format.

A.1.20 *omp.f90*

Routines for switching between global and IJ-block structures. Slightly modified compared to UCI routines, e.g. looping is changed to reduce striding.

- MPSPLIT: Split global arrays into IJ-block arrays.
- MPBIND: Convert back to global arrays.
- get_iiijmp: From global indices I, J, find IJ-block indices II, JJ, MP. Not really necessary because of the array `all_mp_indices` and the next routine:
- get_all_mpind: Sets up array `all_mp_indices` to map global indices to IJ-block indices.
`all_mp_indices(1,I,J)=II`
`all_mp_indices(2,I,J)=JJ`
`all_mp_indices(3,I,J)=MP`

A.1.21 *pbl_mixing.f90*

Routines for calculating planetary boundary layer (PBL) mixing. This is the f90 version of the UCI file *p-pbl.f*, but modified to use the scheme by Holtslag et al. (1990).

- CNVBDL: Main routine for calculating PBL mixing.
- BULK: Prather bulk scheme.
- get_keddy_L1: Calculates diffusivity in the lowermost model layer, as done in the routine KPROF.
- KPROF2: Calculates diffusivity of heat used in PBL closure, as used by the Holtslag et al. (1990) scheme. Should be used instead of KPROF, since unnecessary calculations have been removed.
- KPROF: Calculates diffusivities used in PBL closure, as used by the Holtslag et al. (1990) scheme.
- PHIM: Calculates similarity theory stability correction for momentum.
- PHIH: Calculates similarity theory stability correction for heat.
- TRIDIAG: Solves tri-diagonal system.
- INTERP: Mass weighted interpolation routine to determine PBL profiles from similarity. Ekman solution.
- QXZON: Combines mass boxes into extended zones.
- QZONX: Divides one extended zone into equal-mass boxes.

A.1.22 *pmain.f90*

The main program *pmain.f90* has been modified for the Oslo CTM3. Input routines are changed and also some calls to master routines. There is also an internal chemistry loop of max 15 minutes for the processes mixing/emissions/chemistry/deposition. This is to reduce the large changes imposed by emissions and deposition. For large deposition values, all of a tracer can be removed at the surface if the time step is too long. For a 16 m layer, a deposition velocity of 1.77 cm/s will remove everything in 15 minutes. Linoz calls has been removed.

See Section 4.1.3 for more.

A.1.23 *regridding.f90*

Routines for regridding data.

- **E_GRID**: Regridding of 2D horizontal field. Field must **not** be per area, i.e. concentrations and mixing ratios must be multiplied by area before interpolation, and divided by new area afterwards. Handles emission dataset which include moments (usually not used in Oslo CTM3). **XBEDG** and **XDEDG** may have shift at dateline. **YBEDG** and **YDEDG** must start at 90S.
- **E_GRID_Y**: Regridding of array in meridional direction.
- **TRUNG8**: Convert double precision (**r8**) field from native resolution to degraded horizontal resolution.
- **TRUNG4**: Convert single precision (**r4**) field from native resolution to degraded horizontal resolution.

A.1.24 *source_uci.f90*

- **SOURCE**: Routine for adding emissions to emission array each time step, when treated as a separate process (i.e. not as production term in chemistry). **Not tested with Oslo chemistry.** When treated as chemistry production term, the routine **emis4chem** in *emisdep4chem_oslo.f90* is used (see Appendix A.2.14).

A.1.25 *scavenging_largescale_uci.f90*

Large scale scavenging as described in Section 7.1.1. Some modifications from Oslo CTM3 are implemented.

- **WASH0**: Master routine calling **WASH1** or **WASH2**.
- **WASH1**: Simple UCI wet scavenging routine. Kept for history; should not be used.
- **WASH2**: Routine by Neu and Prather (2012), partly modified for Oslo CTM3.
- **DISGAS**: Calculates the mass of tracer dissolved in aqueous phase. Uses the flag **IT258K** to define how to use Henry's law.
- **HENRYS**: Use Henry's law to calculate mass dissolved in aqueous phase. No dissolved tracer below 258 K, and uses retention coefficient between 258 K and 273 K.
- **HENRYSallT**: Same as **HENRYS**, but uses retention coefficient also below 258 K.
- **RAINGAS**: Calculates tracer (kg) picked up by *new* rain.
- **WASHGAS**: Calculates tracer picked up by falling precipitation (kg) and also evaporated from precipitation (kg).
- **DIAMEMP**: Empirical fit of precipitation diameter to cloud water density and rain rate, following Field and Heymsfield (2003).
- **GAMMAX**: Calculates gamma using \ln gamma algorithm.
- **WETSET_CTM3**: Initialises and sets wet scavenging parameters for Oslo CTM3.

A.1.26 *spectral_routines.f*

Spectral routines, not collected as module. These are purely inherited from UCI/Oslo CTM2.

- **SPE2GP**: Converts spectral field to gridded field.
- **ZD2UV**: Converts spectral fields of vorticity and divergence to gridded field of zonal wind (**U**) and meridional wind (**V**).
- **UVC0EF**: Used by **ZD2UV** to calculate spectral coefficients.
- **FFT_99**: Multiple fast real periodic transform of length **N** performed by removing redundant operations from complex transform length **N**.
- **FFT_RPASS**: Performs one pass-thru data as part of multiple **FFT** (**FFT_99**).
- **FFT_DDSS**: Calculate constant arrays needed for evaluating spectral coefficients for **U** and **V** from vorticity and divergence.
- **FFT_SET**: Computes factors of **N** and trigonometric functions needed by **FFT_99**.
- **LEGGEN**: Calculate Legendre functions.
- **GAUSSST**: Old routine for calculating Gaussian quadrature points and weights. Use **GAUSSST2** (*grid.f90*) instead.

A.1.27 *steflux.f90*

Routines for calculating stratosphere-troposphere exchange (STE) as explained in Section 21.1.4. This is the f90 version of UCI code *p-chemflux.f*.

- **CHEMFLUX**: Saves the horizontal flux of specified tracer (usually **O₃**) in the troposphere, but only for tropospheric to tropospheric boxes.
- **CHEMFLUX_E90**: Finds horizontal fluxes within the troposphere based on e90-tracer.
- **dumpuvflux**: Accumulates horizontal fluxes into 3D arrays. Accumulates over time period defined by flux calendar (**JD0_X**).
- **DUMPTRMAS**: Accumulates tropospheric mass of tracer (**O₃**).
- **DUMPTRMAS_E90**: Accumulates tropospheric mass of tracer (**O₃**) based on e90 tracer.
- **SAVETRMAS**: Saves daily average mass of tracer (**O₃**).
- **STEBGT_CLR**: Clears STE diagnostics.
- **STEBGT_WRITE**: Writes STE budget to netCDF4 file.
- **ctm3_pml**: Calculates tendency (production minus loss; **PML**) below predefined **O₃** surfaces.
- **ctm3_o3scav**: Calculates net scavenged **O₃** below predefined **O₃** surfaces.
- **chemflux_setup**: Set up STE diagnostics.

A.1.28 *stt_save_load.f90*

Contains routines to save and load STT from restart files.

- **load_restart_file**: Restart from netCDF4 files saved by **save_restart_file**. Setting argument **MODE** to zero will read the main restart file (also setting **AIR**), while non-zero will read additional fields from specified files. This has to be hard-coded in the subroutine **SETUP_SPECIES** in the file *initialize.f90*.
- **getField_and_interpolate**: This routine is bound to **load_restart_file**, and reads a 3D field from a netCDF4 file, with **ncid** as file id and **var_id** as variable id. If resolution on file differs from model resolution, the field is interpolated to model resolution. Vertical interpolation is not possible yet.

- **save_restart_file**: Saves netCDF4 restart file. Contains variables necessary for restarting a run, as well as useful variables for other purposes. Transported species have prefix STT_, and for these species there are also moments available, having prefixes SUT_, SVT_, SWT_, SUU_, SVV_, SWW_, SUV_, SUW_, SVW_. Non-transported species have prefix XSTT_.
- **OSLO_CON_RUN**: Restart from files saved by OC_CON_SAV. Setting argument MODE to zero will read the main restart file, while non-zero will read additional fields from any specified file. Must match model resolution.
- **OSLO_CON_SAV**: Old routine for saving restart file; instant fields, component by component. Called based on input file flag JDO_C. The restart file also contains grid info to use when e.g. interpolating to other resolutions. Should not be used.
- **restart_from_CTM3avg**: Starts from Oslo CTM3 *avgsavDDDDD.dta* files, version 7. Reads the file *avgsav_input* (no extension), so you must rename the input file accordingly. Must match model resolution.
- **restart_from_CTM3avg_T42**: Same as **restart_from_CTM3avg**, but reads T42 resolution *avgsavDDDDD* files and interpolates to current resolution. It reads the file *avgsav_input* (no extension).
- **OSLO_CON_RUN42**: Reads Oslo CTM3 T42 resolution restart file, and interpolates to current resolution. Works on sav-files version 1 and 2.
- **OSLO_CON_RUNxx**: Reads any Oslo CTM3 resolution restart file, and interpolates to current resolution. Requires that the sav-file is version 2 or higher. Will stop if model resolution is the same as on file, because not all moments are used.
- **OSLO_RESTARTFILE_INFO**: Retrieves resolution info from the old binary restart files.

A.1.29 *utilities.f90*

Various utilities for Oslo CTM3. More utilities are given in *utilities_oslo.f90*.

- **write_log**: Writes start and end of model to screen.
- **model_info**: Prints info about run to screen.
- **calendar**: Calculates day counters, but also some info about next time step, such as JYEAR_NEXT, JMON_NEXT, JDAY_NEXT, JDATE_NEXT.
- **is_leap**: Calculates whether a year is leap year or not.
- **get_soldecdis**: Calculates solar declination and distance to Sun. Same as originally found in CALENDR.
- **CALENDR_OLD**: Old routine to calculate day counters and also solar declination and distance to Sun. Not used.
- **CALENDL**: Looks up calendar and checks for flags.
- **LOCSZA**: Calculates cosine of local solar zenith angle, and the solar flux factor.
- **LCM**: Calculates the least common multiple of two numbers.
- **ctmExitC**: Exit routine printing message.
- **ctmExitL**: Exit routine printing message and label.
- **ctmExitIJL**: Exit routine printing message and I, J, L.
- **get_free_fileid**: Finds a free file id number.

- **get_dinm**: Returns the number of days in months, depending on whether year is leap year or not.
- **CFRMIN**: Set minimum limit on cloud fraction.
- **CIWMIN**: Set minimum limit on in-cloud water and ice ratios (kg/kg).
- **check_btt**: Checks BTT array for negatives and NaNs. Allows tracer id 110 (sum of oxygen, SO) to be negative.
- **adjust_moments**: Scales down moments if BTT has been reduced during a process (if it is smaller than BTTBCK).

A.1.30 *p-cloud2.f*

Routines for calculating cloud2. Will be updated when cloud-J is included.

- **CLOUD**: Calculates cloud properties.
- **QUADCA**: Generates 4 quadrature independent column atmospheres (ICAs).
- **OD_LIQ**: Sets effective radius and extinction for liquid clouds.
- **CLDQUAD**: Generates independent ICAs from maximum random overlap criteria.
- **QUADM**: Sort ICAs in order of increasing optical depth. Calculates weights.
- **ICANR**: Evaluate number of ICAs.
- **HEAPSRT**: Heap sort.

A.1.31 *p-dyn0.f*

Sets up atmospheric variables after they have been read from file.

- **DYN0**: Sets up advective fields.
- **EPZ_UV**: Redistributes U and V fluxes to smooth over extended polar zones.
- **EPZ_TQ**: Average temperature (T) and specific humidity (Q) over extended polar zones.
- **EPZ_P**: Average surface pressure (P) over extended polar zones.
- **PFILTER**: Global filter to smooth pressure errors. Also adjusts the horizontal fluxes accordingly.
- **CFLADV**: Calculates global Lifshitz (not CFL) time step limiter for advection step. NADV is the number of global advection steps.

A.1.32 *p-dyn0-v2.f*

Same as *p-dyn0.f*, but for more accurate polar cap treatment.

A.1.33 *p-dyn2.f*

Contains advection subroutines.

- **DYN2UL**: Zonal advection.
- **DYN2VL**: Meridional advection.
- **DYN2W_OC**: Vertical advection.
- **QLIMIT2**: Quick SOM limiter only for LIM=2 (pos+mono) in the X direction.
- **POLES1**: Combine polar-pie box with next lower latitude (J=1,2 and J=JM-1, JM) using SOM.
- **POLES2**: Split extended polar-pie box back into two (J=1,2 and J=JM-1, JM). Use SOM to split, need to know final air mass in J=1 and J=JM.

A.1.34 *p-dyn2-v2.f*

Same as *p-dyn2.f*, but for more accurate polar cap treatment. Does not use POLES1 and POLES2. Calls from *pmain.f90* needs to be modified (described in *pmain.f90*).

A.1.35 *p-linoz.f*

Linoz is available in Oslo CTM3, but only for STE calculation (Section 21.1.4). Here are the available routines, but note that some are not used because Linoz is only used for STE.

- LNZ_INIT: Read/init Linoz data and other strat chem tables from pratio box model.
- LNZ_SET: Set up Linoz (and other stratosphere) table data for each day/month/year.
- LNZ_SET03: Initialize Linoz O₃ (N=N_LZ) based on supplied climatology.
- LNZ_PML: Linoz = linearize P-L for stratospheric ozone based on tables from the PRATMO model using climatological T, O₃, Month.
- INT_LAT: Interpolate from pratio standard tables (85S to 85N) to CTM J-grid.
- INT_MID: Interpolation routine, using grid box midpoint.
- INT_SOM: Interpolation routine using moments.
- DECAY: Simple e-fold decay of species throughout the model domain. **Not used; Oslo CTM3 uses its own routine.**
- TPAUSEB: Defines the tropopause level based on Linoz O₃. **Not used; rather use TPAUSEB_E90.**
- TPAUSEG: **Not used; rather use TPAUSE_E90.**

A.1.36 *p-vect3.f*

The second order moment 1D transport routine QVECT3.

A.1.37 *p-phot_oc.f*

Contains the column model for fast-JX, used by the main driver *jv_column* in *main_oslo.f90*.

- PHOT0J: Column model for J-values. T, O₃ and mass is also set from climatology in the uppermost layer (TTJ, DDJ and ZZJ for L1-1).
- OPTICL: Sets cloud fast-JX properties at the std 5 wavelengths (200, 300, 400, 600, 999nm).
- OPTICA: Sets aerosol fast-JX properties at the std 5 wavelengths (200, 300, 400, 600, 999nm).
- OPTICM: Sets fast-JX properties for Mie scattering.
- SOLARZ: Solar zenith angle.
- SPHERE2: Calculation of spherical geometry.
- EXTRAL: Adds sub-layers (JXTRA) to thick cloud/aerosol layers.
- FLINT: Three point linear interpolation function.
- JRATET: Interpolates J-values.
- JP_ATM: Print out atmosphere used in J-value calc
- OPMIE: Mie scattering code.
- MIESCT: Mie scattering, used by OPMIE.
- LEGND0: Calculates ordinary Legendre functions.
- BLKSLV: Sets up and solves the block tri-diagonal system.
- GEN_ID: Generates coefficient matrices for the block tri-diagonal system.
- :

A.2 Oslo source files

The Oslo source files are located in the directory *OSLO*.

A.2.1 *cmn_oslo.f90*

Defines variables needed for Oslo chemistry, which are not part of the transport code. It may be that some of these variables should have been in the other *cmn*-files.

Physical variables:

- LMTROP (IPAR, JPAR): The uppermost level of troposphere. Stratosphere starts at LMTROP+1.
- NEW_TP: Switch used to diagnose the calculated tropopause.
- PARTAREA (LPAR, IPAR, JPAR): Background aerosol surface area density. Be aware that the indexing has changed since Oslo CTM2.

Convective washout variables:

- TCCNVHENRY (NPAR): Flag to decide which Henry constant to use for convective wash out.
- LELEVTEMP (2, IDBLK, JDBLK, MPBLK): Flag for convective plume/elevator temperatures. If minimum plume temperature is below 258 K the first entry is 1, and if maximum temperature is below 273.15 K the second entry is 1. Otherwise these flags are 0.
- QFRAC Fraction of elevator convective precipitation / elevator liquid water volume.
- LW_VOLCONC Convective elevator liquid water volume concentration.

Air values:

- AIRMOLEC_IJ (LPAR, IDBLK, JDBLK, MPBLK): Air density.
- DV_IJ (LPAR, IDBLK, JDBLK, MPBLK): Gridbox volume.

Tracer related variables:

- trsp_idx (TRACER_ID_MAX): Mapping from chemical ID to transport number.
- chem_idx (NPAR) Inverse mapping for trsp_idx (from transport number to chemical ID).
- Xtrsp_idx (TRACER_ID_MAX) Mapping from chemical ID to non-transported number (place in XSST).
- Xchem_idx (NOTRPAR) Reverse mapping for Xtrsp_idx.
- XTNAME (NOTRPAR) Name array for non-transported tracers.
- XTMASS (NOTRPAR) Tracer mass for non-transported tracers.
- XTMASSMIX2MOLMIX (NOTRPAR) Conversion from kg/kg to mole/mole (i.e. M_AIR/XTMASS).
- XTOLMIX2MASSMIX (NOTRPAR) Conversion from mole/mole to kg/kg (i.e. XTMASS/M_AIR).
- XSTT (LPAR, NOTRPAR, IPAR, JPAR): The non-transported tracer distribution.
- XSTTAVG (LPAR, NOTRPAR, IPAR, JPAR): The diagnostic (avgsav) array of the non-transported tracers.

Chemical variables:

- JVAL_IJ (JPPJ, LPAR, IDBLK, JDBLK, MPBLK): J-values.
- STT_2D_LB: Lower boundary conditions for tracers.

- **STT_2D_LT**: Upper boundary conditions for tracers.
- **TROPCHENegO3**(L_{PAR},M_{PBLK}): Counting number of negative O₃ occurring in the troposphere (I have only found this in the surface layer).
- **PR42HET**(I_{PAR},J_{PAR}): Aerosol surface conversion of N₂O₅ to HNO₃.
- **CH4FIELD**(I_{PAR},J_{PAR}): Surface field for CH₄ set each month. Not used when CH₄ emissions are turned on.

Emission variables:

- **EMIS_IJ**(L_{PAR},N_{PAR},I_{DBLK},J_{DBLK},M_{PBLK}): Emissions for Oslo chemistry treatment as production in chemistry, i.e. units [molec/(cm³s)].
- **DIAGEMIS_IJ**: Diagnose emissions accumulated (kg) over time span defined by budget calendar (J_{DO_T}).
- **emisTotalsDaily**(N_{PAR},366): Diagnose daily accumulated emissions (kg).
- **emisTotalsOld**(N_{PAR}): Used for the daily accumulated emissions diagnose.
- **METHANEMIS**: Logical specifying whether CH₄ emissions are to be used or not.
- **NECAT**: Number of emission categories to diagnose (only used for diagnostics).
- **ECATNAMES**(NECAT): 3-character names for each emission category. So far the RETRO categories are used.
- **E2CTBL**(ET_{PAR}): Mapping category number to emission table.
- **E2LocHourTBL**(ET_{PAR}): Table mapping 2D emission table to diurnal variation index. See Section 8.4.2.
- **NE2LocHourVARS**: Number of local hour scalings.
- **E2LocHourSCALE**(24,NECAT,NE2LocHourVARS): Local hour scalings.
- **E22dTBL**(ET_{PAR}): Table mapping 2D emission table to horizontal 2D variation index. See Section 8.4.2.
- **NE22dVARS**: Number of horizontal 2D types.
- **E22dSCALE**(I_{DBLK},J_{DBLK},M_{PBLK},NE22dVARS): 2D scalings.
- **E2L2dTBL**(NE22dVARS): Keep track of 2D scalings used.
- **E2vertTBL**(ET_{PAR}): Table mapping 2D emissions to vertical distributions.
- **NE2vertVARS**: Number of vertical distributions.
- **NE2vertLVS**: Number of vertical levels for the distributions.
- **E2vertSCALE**(NE2vertLVS,NE2vertVARS): The vertical scalings.

Forest fires variables:

- **FF_TYPE**: Type of forest fires emissions.
- **FF_YEAR**: Year of forest fires dataset.
- **FF_PATH**: Path of forest fires, set in *Ltracer_emis_XXX.inp*.
- **NEFIR**: Number of components with forest fires emissions. Must not be larger than E_{PAR_FIR}.
- **E_{PAR_FIR}**: Max number of components with forest fires emissions.
- **E_{PAR_FIR_LM}**: Vertical CTM layers covered.
- **E_{COMP_FIR}**(E_{PAR_FIR}): Components emitted.
- **EMIS_FIR**: The forest fires emission array of size (E_{PAR_FIR_LM},E_{PAR_FIR},I_{DBLK},J_{DBLK},M_{PBLK}).

Global diagnose variables:

- **DIAGEMIS_IJ**: Diagnose emissions accumulated (kg) over time span defined by budget calendar (J_{DO_T}).

- **emisTotalsDaily**(N_{PAR},366): Diagnose daily accumulated emissions (kg).
- **emisTotalsOld**(N_{PAR}): Used for the daily accumulated emissions diagnose.
- **CONVWASHOUT**(L_{PAR},N_{PAR},I_{DBLK},J_{DBLK},M_{PBLK}): Diagnose tracer removed by convective scavenging (kg), accumulated over time span defined by budget calendar (J_{DO_T}).
- **dobson_snapshot**(I_{PAR},J_{PAR},24): Snapshots of total O₃ column each hour (DU).
- **dobson_snapshot_ts**(I_{PAR},J_{PAR},24): Snapshots of tropospheric O₃ column each hour (DU).
- **TEMPAVG**: Temperature average, accumulated over time span defined by budget calendar (J_{DO_T}).
- **H2OAVG**: H₂O average, accumulated over time span defined by budget calendar (J_{DO_T}).
- **QAVG**: Specific humidity average, accumulated over time span defined by budget calendar (J_{DO_T}).
- **AMAVG**: Air density average, accumulated over time span defined by budget calendar (J_{DO_T}).
- **LMTROPAVG**: Average level of tropopause height (LMTROP), accumulated over time span defined by budget calendar (J_{DO_T}).
- **SCAV_LS**: Accumulated amount (kg) removed by large scale scavenging.
- **SCAV_CN**: Accumulated amount (kg) removed by convective scavenging.
- **SCAV_DD**: Accumulated amount (kg) removed by dry deposition.
- **SCAV_BRD**: Accumulated burden to be used for calculating average burden.
- **SCAV_DIAG**(N_{PAR},4,366): Daily accumulated values. Last entry is average burden.
- **SCAV_MAP_WLS**: Total (kg) scavenged by large scale scavenging at the surface.
- **SCAV_MAP_WCN**: Total (kg) scavenged by convective scavenging at the surface.
- **SCAV_MAP_DRY**: Total (kg) scavenged by dry deposition at the surface.

Help variables:

- **DINM**: Number of days in month, changes depending on leap year or not.
- **ZEROINIT**: Flag to keep track of initialised components.
- **XZEROINIT**: Flag to keep track of initialised non-transported components.
- **RESULTDIR**: Can be used to put results in a specified directory.
- **dustbinsradii**: Radius of dust bins. Only set if mineral dust module is included.

A.2.2 aerosols2fastjx.f90

Routine for handling tropospheric aerosols in fast-JX.

- **initialize_tropaerosols**: Initialize arrays.
- **set_aer4fjx**: Calculate the path of each aerosols, to be used in fast-JX calculations.
- **get_tropaerosols**: Reads monthly model climatology for specified aerosols. *Not fully implemented*.
- **update_tropaerosols**: Sets the climatological values of aerosols, interpolates temporally between two monthly climatologies.
- **set_aer4fjx_ctm2**: Sets simple BC profile as in CTM2.

A.2.3 *bcoc_oslo.f90*

Routines for treating the BCOM module (Section 14).

- **bcoc_init**: Initializes the BCOM; indices are set and dry deposition is set.
- **bcoc_master**: Master routine for calculating BCOM. Loops through IJ-blocks and their columns and integrates aerosol masses using QSSA.
- **bcoc_setdrydep**: Puts deposition rates into VDEP. It is called from the routine **setdrydep**. Stability is treated in the latter after VDEP has been set.
- **bcoc_chetinit**: Initialize latitude dependent aging times.
- **bcsnow_init**: Initialize BCsnow.
- **bcsnow_diagwetrm**: Diagnose BC removed by wet scavenging and deposited on snow.
- **bcsnow_save_restart**: Save restart file for BCsnow diagnostics.
- **bcsnow_status**: Print status of BCsnow.
- **bcsnow_check_snow** (private): Debug routine for BCsnow.
- **bcsnow_getspringsummer** (private): Get dates for spring and summer to be used in melting calculations.
- **bcsnow_nmet_output**: Puts BCsnow data to file every NMET.
- **bcsnow_nmet_output_nc**: Puts BCsnow data to netCDF file every NMET.
- **bcsnow_collect_ij** (private): Collects diagnosed amount of BC deposited on snow, from wet scavenging and dry deposition, thus building snow layers.
- **bcsnow_meltevap_ij** (private): Calculates evaporation.
- **bcsnow_seaice_ij** (private): Corrects calculations over sea ice.
- **bcsnow_adjustment_ij** (private): Adjusts calculated snow depth to snow depth from meteorological data.
- **bcsnow_master**: BCsnow master routine.

A.2.4 *caribic2.f90*

Routines for producing vertical profiles at CARIBIC measurement locations and times. CARIBIC input is available from 2005. Called from **nops_diag** in *diagnostics_general.f90*.

- **get_new_events** (private): Find observations for this day.
- **caribic_output** (private): Produces output for the given NOPS and the previous NOPS.
- **caribic_data_to_file** (private): Write collected flight path data to file.
- **caribic2_master**: Process profiles. Called outside parallel region.

A.2.5 *ch4routines.f90*

Routines for treating CH₄ as fixed at surface or as emissions. To choose type of constant surface data, use CH4TYPE at the top of this file. To use emissions, set flag METHANEMIS in *cmn_oslo.f90*.

- **update_ch4surface**: Updates surface mixing ratios. This is mainly done from pmain.

- **ch4surface_hymn** (private): Reads surface data from HYMN, given for years 2003-2005. This is standard.
- **ch4surface_scale_hymn** (private): Scales HYMN 2003 dataset to marine global annual CH₄ observed by ESRL Global Monitoring Division http://www.esrl.noaa.gov/gmd/ccgg/trends_ch4/
- **ch4surface_poet** (private): Reads surface data from POET.
- **ch4surface_retro** (private): Reads surface data from RETRO.
- **READCH4** (private): Carries out the actual read-in for POET data.
- **set_ch4_stt**: Sets 3D CH₄, i.e. in the STT array, to values found in HYMN.
- **updateS0ILUPTAKEbousquet**: Updates soil uptake each month, according to the Bousquet data.
- **read_ch4sfc4soiluptake** (private): Reads HYMN surface data [kg], to convert Bousquet data from [kg/s] to [1/s].
- **read_ch4bousquet** (private): Reads the Bousquet data. Can read any year in dataset, but standard is to read 2003, matching the HYMN surface data for 2003.
- **ch4drydep_bousquet**: Calculates the dry deposition velocity of CH₄ to be used in Oslo CTM3.
- **reportsfcch4**: Reports global average surface mixing ratio of CH₄.
- **setch4sfc**: Set CH₄ at surface to keep it constant.

A.2.6 *chem_oslo.f90*

This is where Oslo chemistry master routine will be located in the future. For now tropospheric chemistry is in *tropchem_oslo.f90* and stratospheric chemistry is in *stratchem_oslo.f90*.

A.2.7 *chem_oslo_rates.f90*

Routines for setting up chemistry reaction rates.

- **TCRATE_CONST2**: Constant rates and rates depending only on temperature. The latter are stored in intervals of 1 K. Rates used in the troposphere are listed first, then the rates only used in the stratosphere are listed.
- **set_pr42het**: Sets aerosol surface uptake reaction for hydrolysis of N₂O₅ in the troposphere. This aerosol climatology is an annual mean height-latitude distribution from (Dentener and Crutzen, 1993), and should be revised.
- **getRQAER** (private): Find removal rate by aerosol (RQAER), only dependent upon land/sea and vertical variation. Crude approximation, should be revised.
- **TCRATE_TP_IJ_TRP**: Rates dependent on temperature and pressure in troposphere.
- **TCRATE_TP_IJ_STR**: Stratospheric rates dependent on temperature and pressure.
- **TCRATE_onAER**: Gaseous uptake and heterogeneous chemistry on aerosols. Includes new and old parameterisations. Tropospheric chemistry.
- **TCRATE_HET_IJ**: Heterogeneous chemistry reactions in the stratosphere.

A.2.8 *cnv_oslo.f90*

Oslo wet removal due to convective rain is treated in two steps:

1. Calculating the fraction of convective rain to cloudwater in the elevator (QFRAC).
2. Calculating the fraction of tracer in cloudwater (DISSOLVEDFRAC).

See Section 6.3 for details. The subroutines in this file are:

- **elevator_fractions**: Calculates QFRAC and LW_VOLCONC. Called from CONVW_OC.
- **liquid_fractions**: Calculates DISSOLVEDFRAC and returns CNV_WETL. Called from CONVW_OC.
- **wf_henry** (private): Calculates Henry coefficients, possibly modified by hard coding.

A.2.9 *dateconv.f90*

Routines for date conversion, used e.g. by *caribic2.f90*.

- **itau2idate**: Calculate date from given time in seconds relative to reference year.
- **idate2itau**: Calculate time in seconds since 1 Jan 1995.
- **julianday**: Calculate julian day from given date.
- **calendardate**: Calculate date from given julian day.

A.2.10 *drydeposition_oslo.f90*

Sets up dry deposition velocities.

- **drydepinit**: Reads *drydep.ctm* from directory *Input_CTM3*.
- **update_drydepvariables**: Sets up special drydep treatments, e.g. soil uptake of CH₄ and variables for the new dry deposition treatment. Called from subroutine **oc_update_chemistry**.
- **setdrydep**: Sets drydeposition velocities each time step, in subroutine **oc_main**.
- **get_ctm2dep** (private): Calculate old (CTM2) treatment dry deposition rates.
- **get_vdep2** (private): Calculate new dry deposition velocities.
- **get_STC** (private): Get monthly mean stomatal conductances.
- **get_PARMEAN** (private): Get monthly mean photosynthetically active radiation (PAR).
- **get_asm24h** (private): Get 24-hour mean of a_{sn} variable for new dry deposition treatment. I.e. daily mean of the molar ratio of SO₂ and NH₃. Uses all NOPS steps to calculate daily mean.

A.2.11 *diagnostics_general.f90*

Oslo chemistry diagnostics. Scavenging diagnostics are located in *diagnostics_scavenging.f90* (Appendix A.2.12).

Variables (private):

- **o3lim**: O₃ mixing ratio used to find tropopause level **tp_o3**, based on where O₃ > **o3lim**.
- **tp_o3**: From surface upwards, this is the uppermost level where O₃ < **o3lim**.

- **preslim**: Pressure limit for hPa-based tropopause **tp_hpa**.
- **tp_hpa**: From surface upwards, this is the uppermost level where p < 100hPa.
- Plus several variables to get running averages of tropospheric OH concentration and CH₄ lifetime.

Subroutines:

- **diag_ohch4n2o_init**: Initializes the lifetime diagnostics.
- **init_lifetime** (private): Initialize CH₄ and N₂O accumulated losses and burdens.
- **du_columns**: Calculate tropospheric and total O₃ columns each meteorological time step.
- **write_ducolumns**: Write the columns to file *dobson_nmet.nc*.
- **init_daily_diag**: Daily initialisations in the beginning of the day.
- **daily_diag_output**: Daily output carried out at the end of the day.
- **nops_diag**: Diagnoses for each NOPS, before parallel loop.
- **mp_diag**: Diagnoses for each IJ-block.
- **TBGT_2FILE**: Processes 2D tendency budgets and dumps to file.
- **REPORTS_CHEMISTRY**: Print out different kinds of reports.
- **sumup_burden_and_lifetimes**: Sum up OH burden and CH₄ lifetime for different tropopause definitions, for a given IJ-block.
- **report_burden_and_lifetime** (private): Print out the burdens and lifetimes.
- **diag_burden_snapshot** (private): Print out burden at specific times.
- **write_snapshot**: Writes out snapshots of selected species/metdata for hemisphere or global. Mass space is put out.
- **write_snapshot_the**: Writes out snapshots of selected species on potential temperature surfaces. Put out as mixing ratio. See Section 21.2.10.
- **ch4n2o_burden2**: Sums up burden of CH₄ and N₂O.
- **ch4_loss3**: Sums up monthly chemical loss of CH₄.
- **n2o_loss3**: Sums up monthly chemical loss of N₂O.
- **ocdiags_tpset**: Sets tropopauses for burden and lifetime diagnostics.
- **report_negO3**: Print out the number of negative O₃ reported by tropospheric chemistry routine.
- **tnd_emis_daily** (private): Saves accumulated emissions for each species per day, in array **emisTotalsDaily**.
- **tnd_emis2file**: Writes the daily emission totals to file *emis_daily_totals_YYYY.nc*. Writing follows the budget calendar, and is called from **pmain**. Also writes accumulated emissions in 3D following the tendency calendar, to file *emis_accumulated_3d_YYYYMMDD_YYYYMMDD.nc*.
- **save_chemPL**: Accumulate chemistry losses, convert to units [kg].
- **chembud_output**: Write chemistry budgets to file. Burden, CHEMLOSS and CHEMPROD, all in units kg/gridbox. Only for selected species. Also see Section 21.2.1.

A.2.12 *diagnostics_scavenging.f90*

Routines for diagnosing dry and wet scavenging.

- **scav_diag_init**: Initialises separate diagnostics for wet scavenging and dry deposition.
- **scav_diag_put_ddep**: Accumulates kg of tracer deposited by dry deposition.
- **scav_diag_brd**: Accumulates burden of tracers each meteorological time step to generate averages.
- **scav_diag_ls**: Diagnose large scale scavenging.
- **scav_diag_cn**: Diagnose convective scavenging.
- **scav_diag_collect_daily**: Collect daily scavenged tracer masses and also the average tracer burden.
- **scav_diag_2fileA**: Write daily totals of scavenged tracer, plus their burdens, to file *scavenging_daily_totals_YYYY.nc*. Scavenging includes wet removal (large scale and convective) and dry deposition.
- **scav_diag_2fileB**: Write 2D daily totals of scavenged tracer (i.e. maps) to file *scavenging_daily_2d_YYYYMMDD.nc*. Scavenging includes wet removal (large scale and convective) and dry deposition.

A.2.13 *dust_oslo.f90*

Routines for treating the DUST module (Section 15).

- **dust_init**: Initializes the DUST.
- **dustinput_met**: Special input for dust calculations.
- **SWradbdg_get** (private): calculate approximatel solar radiation in and out at the surface. Not used when available from meteorological data.
- **psadjust** (private): Adjust Ps, account for advection.
- **dust_globalupdate**: Update global DUST parameters.
- **oro_set** (private): Set orography.
- **plevs0** (private): Get pressure, temperature and height properties for DUST.
- **dust_master**: Master routine for calculating DUST. Calls column solver for DUST.
- **dust_column** (private): Column treatment of DUST; calls DEAD routines to solve DUST in the column.
- **dustbdg2d**: Writes dust budget to file.
- **dist_set_ssr**: Sets meteorological variable SSRD in dust code.
- **dist_set_strd**: Sets meteorological variable STRD in dust code.
- **dist_set_SWL1**: Sets meteorological variable SWL1 in dust code.
- **dustbdg2file**: Puts out dust budget to netCDF file.

A.2.14 *emisdep4chem_oslo.f90*

Routines to treat get emissions and deposition values and convert them for use in chemistry as production and loss terms, respectively.

- **emis4chem**: Routine similar to the core **SOURCE**, fetching all emissions from the emissions array (as kg/s). The output array is **EMIS_IJ**(**IPAR**,**NPAR**,**IDBLK**,**JDBLK**,**MPBLK**).

- **getEMISX**: Fetches the column emissions for all chemical IDs, converts from kg/s to molec/(cm³s) and puts them into **EMISX**(**TRACER_ID_MAX**,**IPAR**). Called from chemistry master routine where column values are retrieved.
- **getVDEP_oslo**: Converts **VDEP**(**NPAR**,**IPAR**,**JPAR**) [m/s] to **VDEP_OSLO**(**TRACER_ID_MAX**) [1/s] to use as loss term in chemistry. See Section 7.2 for more.

A.2.15 *emissions_aircraft.f90*

Routines for reading and updating aircraft emissions. Possible datasets cover TradeOff, React4C and Quantify. In the *Ltracer_emis_XXX.inp*, you specify **AirScen** to define the dataset, and **AirEmisPath** to define the path to where aircraft emissions are in general.

Emissions are interpolated to the model resolution. Old routines are also available for having the possibility to read old resolution specific emission data. Emissions are read into a separate array, which is used either in **SOURCE** or in **emis4chem**.

- **aircraft_emis_master**: Master routine for treating aircraft emissions.
- **aircraft_set_species**: Defines which species to emit.
- **aircraft_emis_update** (private): Read data from file.
- **aircraft_emis_vinterp** (private): Vertical interpolation.
- **ac_interp** (private): Interpolation routine used by **aircraft_emis_vinterp**.
- **read_original_res** (private): Read original (e.g. 1x1 degree) data.
- **read_tradeoff_original** (private): Read original TradeOff data.
- **read_react4c_original** (private): Read original React4C data.
- **read_quantify_original** (private): Read Quantify data.
- **readmass_qfyAIR_month** (private): Routine to do the netCDF reading of Quantify data, called by **read_quantify_original**.
- **read_ceds_original** (private): Read CEDS data.
- **get_xyedges** (private): Get grid box info for interpolation.
- **aircraft_zero_400hpa** (private): Below 400 hPa, zero out the aircraft tracers (H₂O). This is done by assuming 1 hour lifetime. Setting to zero may cause negative tracers due to moments not being zeroed.

It should be possible to include a diurnal variation for aircraft emissions, but it has not been implemented yet.

A.2.16 *emissions_megan.f90*

Contains routines for calculating MEGANv2.10 emissions (Guenther et al., 2012). Oslo CTM3 routines are:

- **megan_report**: reports daily totals of MEGAN. Should not be included as default.
- **add_meganBiogenic**: Adds MEGAN emissions to species in Oslo CTM3.
- **megan_get_co2**: Reads file to get monthly CO₂ for isoprene activity factor.

- **megan_input:** Reads input table *tables/megan_tables.dat*.
- **megan_update_metdata:** Updates meteorological data needed in MEGAN (e.g. accumulated rain). Also sets monthly CO₂.
- **megan_emis:** Main routine for calculating emissions.
- **getWP:** Get wilting point for soil.
- **megan_emis2file:** Puts emitted amounts to file following the BUDGETS calendar. See Section 8.6.2.

MEGAN routines adjusted to Oslo CTM3:

- **GAMMA_AGE:** Calculate leaf age activity.
- **GAMMA_CANOPY:** Calculate activity from canopy.
- **DISTOMATA:** Calculate drought-induced effect on stomata (range 0–1) based on the Palmer Severity Drought Index. Note that MEGAN sets the drought index to zero as default.
- **Ea1t99:** Temperature dependence activity factor for emission type 1 (e.g. isoprene, MBO).
- **Ea1ti99:** Calculate light independent algorithms.
- **Ea1p99:** Not sure what this does.
- **WaterVapPres:** Convert water mixing ratio (kg/kg) to water vapor pressure.
- **Stability:** Temperature lapse rate in canopy, using canopy characteristics and solar input.
- **GaussianIntegration:** Gaussian distribution.
- **SolarFractions:** Calculate transmission, the fraction of photosynthetic photon flux density (PPFD) that is diffuse, and fraction of solar rad that is PPFD.
- **WeightSLW:** Calculates a gaussian weighting function for LAI in the canopy layers.
- **CanopyRad:** Canopy light environment model.
- **CalcExtCoeff:** Calculates extinction coefficient.
- **CalcRadComponents:** Radiative calculations.
- **CanopyEB:** Canopy energy balance model for estimating leaf temperature.
- **LeafEB:** Leaf energy balance.
- **ConvertHumidityPa2kgm3:** Convert Pa to kg/m³.
- **ResSC:** Leaf stomatal resistance. Not well referenced.
- **LeafIROut:** IR thermal radiation energy output by leaf.
- **LHV:** Calculate latent heat of vaporisation from Stull (1988), p.641.
- **LeafLE:** Latent energy term in energy balance.
- **LeafBLC:** Boundary layer conductance.
- **LeafH:** Convective energy term in energy balance (W/m² heat flux from both sides of leaf).
- **SvdTk:** Calculate saturation vapor density.
- **CalcEccentricity:** Calculate eccentricity.
- **UnexposedLeafIRin:** Calculate IR into leaf that is not exposed to the sky.
- **ExposedLeafIRin:** Calculate IR into leaf that is exposed to the sky.
- **SOILNOX:** Calculation of soil NO_x based on Yienger and II (1995).
- **FERTILZ_ADJ:** Computes fertilizer adjustment factor for soil NO_x.
- **GROWSEASON:** Computes day of growing season for soil NO_x.
- **prec_adj:** Calculates precipitation pulse adjustment factor for soil NO_x.
- **getPulseType:** Computes the pulse type from a rainfall rate (Yienger and II, 1995).
- **precipfact:** Computes a precipitation adjustment factor.

A.2.17 *emissions_ocean.f90*

Routines for treating emissions from ocean. Also sea spray routines will be placed here eventually.

- **emissions_ocean_organiccarbon_init:** Initialise variables for using oceanic emissions.
- **emissions_ocean_getChlA:** Fetches chlorophyll A for specified month. Uses MODIS chlorophyll A, which has been binned into 0.5x0.5 degree grid. Uses meteorological year for years 2003–2012, and otherwise a climatology of those years.
- **emissions_ocean_organiccarbon:** Calculate emissions of oceanic organic carbon aerosols (POA), following Gantt et al. (2015). If sea salt module is included, use sea salt production rate, otherwise calculate it separately (slightly different method for now). This routine only depend on meteorological variables, and is called from **update_emis_ii** (*emissions_oslo.f90*).
- **emissions_ocean_total:** Print out current total POA flux as [Tg/yr].
- **add_oceanOCemis:** Routine to add oceanic carbon emissions. Called from either **emis4chem_oslo** or **SOURCE**.

A.2.18 *emissions_oslo.f90*

Routine for reading in emissions, and master routine for short term variations.

- **emis_input:** Reads in emission data based on *Ltracer_emis_***.inp*.
- **update_emis:** Updates short term variations/emissions globally.
- **update_emis_ij:** Update short term emissions in an IJ-block.
- **emis_prop** (private): Set properties for input data.
- **emis_unit** (private): Unit conversions for datasets.
- **emis_check2dscale** (private): Check 2D scaling flag and keep track of which ones are used.

A.2.19 *emissions_volcanoes.f90*

Variables and routines for volcanic emissions.

Variables:

- **volc_emis_so2:** Emissions of SO₂ for each event.
- **volc_elev:** Elevation of the volcano.
- **volc_cch:** Cloud column height, i.e. the height of the cloud rising from the volcano. When equal to the elevation, the volcano is non-eruptive, i.e. gassing from the surface.
- **volc_ii:** IJ-array zonal index of event.
- **volc_jj:** IJ-array meridional index of event.
- **volc_mp:** IJ-array number.
- **volc_event_start(31,12):** Keeps track of first event for each day, through the year.
- **volc_event_end(31,12):** Keeps track of last event for each day, through the year.

Subroutines:

- **init_volcPATH:** Initialize file path and year for volcanic emissions.

- **read_volcEMIS**: Master routine for reading volcanic emissions.
- **read_volcEMIS_HTAP**: Reads HTAP volcanic emissions (1979–2010).
- **read_volcEMIS_ACOM**: Reads AEROCOM volcanic emissions.
- **add_volcEMIS**: Adds volcanic SO₂ emissions to emission array.

A.2.20 *emisutils_oslo.f90*

Routines used by *emissions_oslo.f90*. When including new types of emissions/datasets, new read-in routines should be placed here.

- **reademis_2d**: Controls the read-in of 2D emission data and its interpolations. This is where you will find info on the 2D format codes used in the emission file *Ltracer_emis_***.inp*.
- **reademis_3d**: Controls the read-in of 3D emission data and its interpolations. This is where you will find info on the 3D format codes used in the emission file *Ltracer_emis_***.inp*.
- **reademis_stv**: Controls the read-in and interpolation of 2D fields used for short term variations (see Section 8.4.4). This is where you will find info on the STV format codes used in the emission file *Ltracer_emis_***.inp*.
- **emisinterp2d** (private): Interpolates 2D field and designates dataset numbers.
- **emis_setscalings**: Set scalingd for tracers using different datasets.
- **scale_area** (private): Scales with dataset by grid box area.
- **get_xyedges**: Calculate grid box properties.
- **set_diurnal_scalings**: Sets simple diurnal scalings. These are e.g. from TNO/RETRO or such as 50 % up in daytime and 50 % down during night.
- **emis_setscaling_2dfields**: Reads scaling data to use for 2D scaling, e.g. daylight temperatures or heating-degree-days.
- **emis_diag**: Accumulates the emissions of each species into DIAGEMIS_IJ.
- **ctm2_rdmolec2** (private): Reads CTM2 POET format.
- **iiasa_read2d** (private): Reads IIASA 2D data as in CTM2.
- **gfed_read3d**: Reads GFED 3D data. Not used in the GFED emissions now; this routine was used to read monthly emissions into the core emission array.
- **volc_read1** (private): Reads volcanic emissions.
- **read_retrobh** (private): Reads the vertical distribution of forest fires.
- **read_bcoc_bond_2d**: Reads Tami Bond data version 4 and 5.
- **read_aerocom_2d**: Reads ascii data from AEROCOM.
- **gfed4_rd**: Reads monthly GFEDv4 data along with partitionings.
- **gfed4_init**: Reads emission factors from GFEDv4.
- **gfed4_rd_novert**: Reads monthly GFEDv4 emissions for distributing according to boundary layer height.
- **gfed4_rd_novert_daily**: Reads monthly GFEDv4 emissions along with daily fraction of emissions per month.

A.2.21 *eqsam_v03d.f90*

Subroutine **eqsam_v03d_sub** is the main nitrate (eqsam) driver, based on Metzger et al. (2002).

A.2.22 *fallingaerosols.f90*

Contains routines for calculating gravitational settling of aerosol using second order moments transport. Not used yet.

- **aerosolsettling**: Master routine.
- **readkasten1968**: Reads aerosol fall speeds of Kasten (1968).
- **getGAMAAER**: The vertical velocity of particles are found based on their radius. Assumes fixed radius for the whole IJ-block.
- **GRAV_SETN**: Routine for SOM transport of a tracer downwards.
- **fallspeed**: Purpose: Given size and density of particle, and column thermodynamic profile, compute terminal fall speed. Based on DEAD/DUST code.
- **turbfallspeed**: Purpose: Given size and density of particle, and column thermodynamic profile, compute Based on DEAD/DUST code.
- **getGAMAAER_NS**: Same as **getGAMAAER** but handles different radii and vertical properties.

A.2.23 *gmdump3hrs.f90*

Routine for dumping selected components to netCDF file every 3 hours. Turn on this diagnose by setting its flag **LDUMP3HRS=.true.**

- **dump3hrs**: Dumps the components.
- **gm_dump_nc** (private): Does the writing to netCDF files. Converts from kg/gridbox to kg/m³.

A.2.24 *hippo.f90*

Routines for producing vertical profiles at HIPPO measurement locations and times. Called from **nops_diag** in *diagnostics_general.f90*.

- **get_new_events** (private): Find observations for this day.
- **hippo_output** (private): Produces output for the given NOPS and the previous NOPS.
- **hippo_data_to_file** (private): Write collected flight path data to file.
- **hippo_master**: Process profiles. Called outside parallel region.

A.2.25 *input_oslo.f90*

Subroutines to initialize the Oslo CTM3.

- **clear_oslo_variables**: Clear arrays used by chemistry (e.g. **trsp_idx**). Called by routine **INPUT**.
- **init_oslo**: Initialize Oslo chemistry. Tracer related data is read, and constant chemical reaction rates are set. Dry deposition parameters are read and some diagnostics are also initialized.
- **info_oslo** (private): Print out info about Oslo chemistry.

- **info_qssa** (private): Print out info about QSSA solver.
- **read_tracer_list** (private): Read tracer list, initialize Oslo chemistry.
- **tracer_specific_input** (private): Read in the tracer-specific run instructions and data sets. Based on UCI CHEM_IN, but set up for Oslo chemistry.
- **set_resultdir** (private): Sets a result directory if defined.
- **read_lsmask**: Reads the land-sea mask LSMASK.

A.2.26 *main_oslo.f90*

The module **main_oslo** comprises the master subroutine for chemistry and aerosol packages.

- **master_oslo**: Master routine to control Oslo chemistry. Processes for each IJ-block is called separately.
- **jvalues_oslo** (private): Collects J-values in the IJ-block.
- **jv_column** (private): Sets photolysis rates in the column. Based on UCI subroutine PHOTOL.
- **update_chemistry**: Update chemistry, e.g. boundary conditions.

A.2.27 *ncutils.f90*

Contains netCDF utilities.

- **readnc_3d_from4d**: Read netCDF file containing 4D fields (DIM1,DIM2,DIM3,DIM4), and returns 3D-field for a DIM4 entry.
- **readnc_2d_from3d**: Read netCDF file containing 3D fields (DIM1,DIM2,DIM3), and returns 2D-field for a DIM3 entry.
- **readnc_1d**: Opens a netCDF file and returns a 1D field of specified size from the file.
- **readnc_1d_from2d**: Opens a netCDF file and extracts a 1D from a 2D field on file. Specifying an entry of DIM2, a 1D array is returned from the 2D array (DIM1,DIM2).
- **get_netcdf_var_1d**: Reads 1D variable from netCDF file. Array is allocated in this routine, and must be deallocated after use.
- **get_netcdf_var_2d**: Reads 2D variable from netCDF file. Array is allocated in this routine, and must be deallocated after use.
- **get_netcdf_var_3d**: Reads 3D variable from netCDF file. Array is allocated in this routine, and must be deallocated after use.
- **get_netcdf_var_4d**: Reads 4D variable from netCDF file. Array is allocated in this routine, and must be deallocated after use.
- **get_netcdf_att_char**: Reads attribute data for variable from netCDF file.
- **get_netcdf_var_dims**: Reads dimensions of variable from netCDF file.
- **get_netcdf_r4var_1d_from2d**: Returns single precision (r4) 1D array from a 2D netCDF field. Used for reading meteorological data on netCDF format.
- **get_netcdf_r4var_2d_from3d**: Returns single precision (r4) 2D array from a 3D netCDF field. Used for reading meteorological data on netCDF format.

- **get_netcdf_r4var_3d_from4d**: Returns single precision (r4) 3D array from a 4D netCDF field. Used for reading meteorological data on netCDF format.
- **handle_err**: Handle netCDF errors. This routine does not print out much helpful information.
- **handle_error**: Handle netCDF errors slightly better than **handle_err**.

A.2.28 *nitrate.f90*

Nitrate routines. Note that the nitrate equilibrium model is located in its own file *eqsam_v03d.f90*.

- **nitrate_init**: Initialise nitrate module.
- **nitrate_master**: Nitrate master routine.

A.2.29 *pchemc_ij.f90*

The tropospheric 1D chemical integrator, integrating the chemistry in the tropospheric column.

The Oslo chemistry was originally set up to use emissions as production terms and deposition as loss terms. This is still default, and is controlled by the user settings in *Makefile* (Section 2.7.1). Note that treating them in chemistry, the lightning and aircraft emissions are also included in the emission array. See Section A.2.14 for more.

A.2.30 *pchemc_str_ij.f90*

The stratospheric 1D chemical integrator, integrating the chemistry in the stratospheric column.

A.2.31 *physics_oslo.f90*

The module **physics_oslo** contains subroutines for doing physical calculations in the Oslo CTM3. Parameters and variables are

- **NTHE**: number of theta levels to calculate equivalent latitudes.
- **pvthe**: Potential vorticity on the theta levels.
- **theqlat**: Equivalent latitude on the theta levels.

The subroutines are

- **update_physics**: Updates physical variables such as tropopause level.
- **defineTP**: Defines the tropopause level, based on the parameter TP_TYPE=1 in *cmn_oslo.f90*. Default for the Oslo CTM3 is a PVU-based tropopause:
- **tp_pvu_ij** (private): Calculates the tropopause level from PVU and potential temperature (TP_TYPE=1).
- **tp_dtdz_ij** (private): Not tested. Calculate the tropopause level using lapse rate (TP_TYPE=2).
- **tp_e90_ij** (private): Not tested. Uses tropopause level from E90 tracer, i.e. as given in LPAUZTOP (TP_TYPE=3).
- **tp_03_150** (private): Not in use. Tropopause based on where O₃ < 150ppbv.

- **get_pvu**: If the meteorological data do not provide PV, it may be calculated from the winds in this routine.
- **ijlw2lij**: Converts a field of size (IPARW,JPAPW,LPARW) to the possibly degraded and vertically collapsed (LPAR,IPAR,JPAP).
- **theta_pv**: Interpolate PV to pre-defined theta levels.
- **theta_eqlat**: Calculates equivalent latitudes for pre-defined theta levels.
- **IJLfield2ThetaLvs**: Interpolates standard IJL-field to θ -levels.
- **metdata_ij**: Sets arrays of air molecular density AIRMOLEC_IJ and box volume DV_IJ. They are used in converting to concentration.
- **check_lmtrp** (private): If E90 tracer needs to be initialised, LMTRP must be defined. If LMTRP is calculated from E90-tropopause, it must be set in another fashion, and for this the PVU tropopause is used. Only carried out at the first time step.

A.2.32 *psc_microphysics.f90*

Variables and routines to calculate formation and evolution of PSCs. Some important variables:

- **N_B**: The number of PSC particle bins.
- **LAEROSOL**: Flag to include aerosol heterogeneous chemistry (in stratosphere).
- **LPSC**: Flag to include PSC1 heterogeneous chemistry.
- **LPSC2**: Flag to include PSC2 heterogeneous chemistry. Requires **LPSC=.true.**
- **PSC1**: PSC1 surface area density.
- **PSC2**: PSC2 surface area density.
- **VOLA**: Volume of frozen aerosols.
- **SAT**: Flags when STS have frozen to NAT.
- **SPS_PARTAREA**: Surface area density of aerosols after PSC modification

And subroutines:

- **oslochem_psc**: Master routine.
- **get_psc12_sad**: Get column values of PSC1, PSC2 and SAD.
- **get_mw**: Fetches coefficients for mass to concentration conversion.
- **PSC_1d_07**: Column model for PSC surface area calculation.
- **CARS**: Carslaw routine.
- **H2O_SAT**: Calculate saturation concentration of H₂O.
- **WSED**: Get falling speed of aerosols.
- **sedimentation**: Sedimentation routine.
- **SED**: Old sedimentation routine
- **AM_BIN**: Calculate H₂O in binary solution.
- **X_CARS**: Used by **AM_BIN**.
- **HENRIC**: Calculate Henry's law constants.
- **RHO_S_CAR**: Calculate density of H₂SO₄ in binary solution.
- **RHO_N_CAR**: Calculate density of HNO₃ in binary solution.
- **LOGN**: Get log-normal distribution.
- **MOM**: Calculate moments of distribution.
- **DIS_LN**: Routine for calling LOGN and MOM.

- **sps_SURF**: Calculate H₂SO₄ mixing ratio from aerosol surface area density.
- **sps_WSASAS**: Get H₂SO₄ mass fraction in a solution with plane surface, and in equilibrium with ambient water vapor pressure.
- **sps_ROSAS**: Get density of the sulphuric acid solution.
- **PSC_diagnose**: Simple diagnostic of PSCs.
- **set_psc_constants**: Initializes the PSC constants.
- **getTnat**: Calculate T_{NAT}, the freezing temperature of NAT.

A.2.33 *qssa_integrator.f90*

Routine for integrating chemistry.

- **qssa**: Integrates chemistry.
- **qssastr**: Same as **qssa**, but allows negative production due to the treatment of the sum of oxygen (SO).

A.2.34 *satelliteprofiles_mls.f90*

Routines for diagnosing satellite profile measurements. Called from **nops_diag** in *diagnostics_general.f90*.

- **get_satprofiles_mls** (private): Get profiles for specified time step.
- **initialize_satprofiles_mls** (private): Initialize.
- **satprofs_mls_to_file** (private): Write to file.
- **satprofs_mls_master**: Control the other routines.

A.2.35 *seasalt.f90*

Routines for treating the SALT module (Section 16).

- **seasalt_init**: Initializes the SALT.
- **seasalt_master**: Master routine for calculating SALT.
- **dry2wet** (private): Calculate the density and diameter of wet sea salt particles.
- **growth_factor** (private): Calculate growth factor.
- **falling** (private): Gravitational settling.
- **drydeppart** (private): Dry deposition.
- **addtogether** (private): Add the parts together.
- **saltbdg2file**: Puts out salt budget to netCDF file.

A.2.36 *seasaltprod.f90*

Contains different sea salt production routines. They are used by both the SALT application and the BCOC application.

- **seasalt_production**: The standard Oslo CTM3 sea salt production, using small particles as in Monahan et al. (1986) as suggested by Gong et al. (1997), and large particles as in Smith et al. (1993).
- **seasalt_production_maartenson03**: Sea salt production following Mårtensson et al. (2003).
- **seasalt_production_gantt15**: Sea salt production following Gantt et al. (2015), i.e. parameterisation of Gong (2003) with sea surface temperature adjustment as in Jaeglé et al. (2011).

A.2.37 *soa_oslo.f90*

Routines for calculating secondary organic aerosols (SOA).

- **soa_init**: Initialise SOA.
- **soa_setdrydep**: Set dry deposition for SOA.
- **SOA_v9_separate**: Master routine for calculating SOA separation, i.e. the amount in gas phase and in aerosol phase.
- **FINDM0** (private): Find concentration of total organic aerosol.
- **FMO**: Used by FINDM0.
- **soa_diag_drydep**: Diagnose SOA drydep.
- **soa_diag_separate**: Diagnose changes in SOA due to separation routine.
- **soa_diag2file**: Writes SOA diagnostics to file.
- **soa_nopsdiag**: SOA diagnoses each NOPS.
- **soa_diag_lsscav**: Diagnose SOA large scale scavenging.

A.2.38 *strat_aerosols.f90*

Routines for setting stratospheric aerosols, i.e. the variable PARTAREA. Aerosol dataset was made by Considine at NASA.

- **update_strat_backaer**: Update background aerosols by adjusting to meteorology.
- **update_ba**: Update background aerosols. Done every month.
- **ctm2_set_partarea**: Adjust satellite data to meteorology, mainly pressure. Assumes that SAD data are means on geographical latitude (i.e. not equivalent latitude).
- **ctm2_set_partarea5**: If a zonal mean dataset uses equivalent latitudes, it is possible to interpolate those to the model by using the model equivalent latitude. This routine tries to do that, but is not in use.
- **meri_interpol**: Interpolate linearly in latitude.

A.2.39 *strat_h2o.f90*

Module for H₂O treatment in the stratosphere. Also sets H₂O in the troposphere.

Variables and parameters:

- **sumH2**: Sum of H₂+2CH₄+H₂O in the stratosphere, as volume mixing ratio.
- **LOLD_H2OTREATMENT**: .true. means H₂O is calculated from the sumH2 (old treatment). .false. means H₂O is calculated in the chemistry, and requires H₂, H₂O and H₂O_s to be transported.
- **str_h2o**: Array containing stratospheric H₂O when calculating from the sum.
- **d_h2o**: Sedimented ice from PSC microphysics.

Subroutines:

- **set_trop_h2o_b4trsp_clim**: Sets tropospheric H₂O values before transport based on model climatology.
- **reset_trop_h2o**: Resets tropospheric H₂O to values from specific humidity.

- **set_strat_h2o_b4chem**: For old treatment, this calculates H₂O from sumH2.
- **set_d_h2o**: Sets **d_h2o**, called from PSC microphysics.
- **strat_h2o_init**: Initialize arrays for H₂O treatment. Will overwrite a possible stored field if H₂O is transported.
- **strat_h2o_abc**: Set upper boundary conditions for H₂O.
- **strat_h2o_abc2**: Set upper boundary conditions for H₂O and H₂ using same mixing ratio as layer below.
- **strat_h2o_max**: Report max H₂O in the stratosphere.
- **zc_strh2o**: Put H₂O into ZC_LOCAL before chemistry if H₂O is not transported.
- **set_h2_eurohydros**: Sets H₂ based on monthly means from the EUROHYDROS project.
- **strat_h2o_init_clim**: Initialise tropopause mixing ratio of H₂ used as climatology.

A.2.40 *strat_loss.f90*

Subroutines:

- **stratloss_oslo**: Stratospheric loss of tracers not handled by stratospheric chemistry routine.

A.2.41 *strat_o3noy_clim.f90*

When calculating only tropospheric chemistry, the module **strat_o3noy_clim** sets up stratospheric O₃, NO_x and HNO₃.

- **read_o3clim**: Reads netCDF file with climatologies of O₃, HNO₃, PANX, HO₂NO₂, NO₃, N₂O₅, NO and NO₂, based on a Oslo CTM2 T42L60 simulation. Reads monthly mean for current and next month.
- **get_strato3noy_clim**: Main routine for non-parallel region. Called 00UTC each day.
- **stratO3_interp** (private): Interpolates linearly in time between two monthly means of climatology, called from **get_strato3noy_clim** once each day.
- **update_stratO3**: Sets O₃ from time interpolated monthly mean climatology. Routine works in parallel over IJ-blocks!
- **stratNOy_interp** (private): Interpolates NO_y components linearly in time between two monthly means of climatology, called from **get_strato3noy_clim** once each day.
- **update_stratNOx** (private): Sets NO_x and HNO₃ similar to Oslo CTM2. Should **not** be used.
- **update_stratNOx2** (private): Inert stratospheric NO_x and HNO₃ are scaled to the NO_x and HNO₃ values used in Oslo CTM2. Should **not** be used.
- **update_stratNOy** (private): Updates stratospheric NO_x and HNO₃ based on the climatology.
- **update_strato3ctm2** (private): Old CTM2 routine for L40. Updates stratospheric O₃ in the uppermost layer assuming an influx of O₃. HNO₃ and NO are set in the stratospheric domain, based on O₃. Should be replaced with an interpolation to L60 climatology.

A.2.42 *stratchem_oslo.f90*

The module `stratchem_oslo` sets up the stratospheric chemistry and calls `OSLO_CHEM_STR` located in *pchemc_str_ij.f90*.

- `oslochem_strat`: Master routine for stratospheric chemistry.
- `read_oslo2d2`: Reads original output from Oslo 2D model and interpolates on the fly. Data are read in `STT_2D_LT` for upper layer (T for top) and `STT_2D_LB` for bottom (B).
- `update_strat_boundaries`: Updates BTT from `STT_2D_LT` at surface and `STT_2D_LB` at model top.
- `set_fam_in_trop`: Sums up stratospheric families in the troposphere.

A.2.43 *sulphur_oslo.f90*

Contains a few variables, and also the ocean concentration of DMS, in the variable `DMSseaconc`.

- `TCRATE_CONST_S`: Sets constant reaction rates for sulphur chemistry.
- `TCRATE_TP_S_IJ`: Calculates heterogeneous reaction rates for sulphur chemistry.

A.2.44 *troccinox_xxx.f90*

Routines for producing vertical profiles at TROCCI-NOX2 measurement locations and times, from January 2005 to early March 2005. 'xxx' is 'fal' for Falcon, 'geo' for Geophysica and 'ban' for Bandeirante. These files are practically identical, and routines are: Called from `nops_diag` in *diagnostics_general.f90*.

- `get_new_events`:
- `flight_output`:
- `flight_data_to_file`:
- `troccixxx_master`:

A.2.45 *tropchem_oslo.f90*

The module `tropchem_oslo` takes care of the tropospheric chemistry calls in the IJ-block. It calls `OSLO_CHEM` located in *pchemc_ij.f90*.

- `oslochem_trop`: Master routine for tropospheric chemistry.

A.2.46 *utilities_oslo.f90*

Contains utilities for the Oslo CTM3, mainly related to Oslo chemistry.

- `gotoZC_IJ`: Put BTT into a local column array for all tracers, indexed by tracer IDs.
- `backfromZC_IJ`: Convert local tracer array back to BTT.
- `ZC_MASS2CONC`: Convert local tracer array from mass to concentration.
- `ZC_CONC2MASS`: Convert local tracer array back to mass.
- `troe`: Old routine to calculate reaction rates for three body reactions.

- `rate3b`: Calculate reaction rates for three-body reactions. Used in both troposphere and stratosphere.
- `get_chmcycles`: Find number of internal loops (CHMCYCLES) for chemistry/boundary layer mixing.
- `US76_Atmosphere`: Compute properties of the 1976 standard atmosphere.
- `h2o_sat`: Calculate saturation concentration of H₂O at a given temperature.
- `source_e90`: Calculate source for e90 tracer.
- `decay_e90`: Calculate decay for e90 tracer.
- `init_e90`: Initialise e90 tracer.
- `tpause_e90`: Find tropopause based on e90 tracer.
- `tpauseb_e90`: Find tropopause in IJ-block based on e90 tracer.
- `tpauseb_o3`: Find tropopause in IJ-block based on Linoz O₃ isopleths.
- `SZA_PN`: Calculates solar zenith angle and also whether it is polar night (PN), i.e. when sun does not go above the horizon.
- `stringUpCase`: Changes a string to upper case letters (English alphabet only).

A.2.47 *verticalprofiles_stations2.f90*

Routines for diagnosing vertical profiles at stations. Called from `nops_diag` in *diagnostics_general.f90*.

- `vprof_stations` (private): Get profiles for specified time step.
- `initialize_stations` (private): Initialize.
- `vprofs_to_file` (private): Write to file.
- `vprofs_master`: Control the other routines.

A.3 DUST source code

The mineral DUST code is located in the directory *OSLO/DEAD_COLUMN*.

A.4 Oslo dummy files

When the Oslo CTM3 is compiled without Oslo chemistry, i.e. run in transport mode only, the Oslo modules used by the core source are replaced with dummy modules in Makefile. The code is designed so that there are very few such files, and further development should also keep such files at a minimum. The files are located in the directory *OSLO/DUMMIES*.

B SVN – Subversion

The Oslo CTM3 is available through the UiO central subversion system (SVN). To access the code you have to be member of the group `gf-ozone`.

SVN is a version control system, and a good introduction is the SVN book, available at <http://svnbook.red-bean.com/>.

To use SVN you need to have SVN installed/loaded. If it is not installed on the computer, it could be available as a module which you can usually load it with

module load svn

Important SVN commands are `checkout`, `add`, `delete/remove`, `commit`, `status`, `diff`.

For version 1.5 you also have `resolve`, which differs from previous versions using `resolved`. You can find documentation of earlier versions on the SVN book home page.

B.1 Repository structure

Only the Oslo CTM3 code, i.e. the `ctm3f90` of SVN, is described in this manual. But there are other tools available through SVN, given in different directories of the repository. One of the most important ones is `utilities`. When you are experienced enough to use branches and tags, you have separate directories for them.

```
ctm3f90/      (Oslo CTM3 code)
MANUAL/      (this manual)
  LATEX/      (latex code manual)
OSLO/        (Oslo chemistry code)
  DEAD_COLUMN/ (Dust code)
  DUMMIES/    (Dummy routines)
tables/      (tables)
  PMEAN/      (to generate annual mean sfcP)
tmp/         (where .o-files end up)
mod/         (where .mod-files end up)
branches/
tags/
utilities/
  generateOpenIFS/
  fast_jx/
    scattering/
      fj_phase/
        mishchenko/
          xsection/
fortran/
  ec2netcdf4/
  generate_ctm3_restart/
idl/
matlab/
ctm2/        (old CTM2 code)
trunk/       ("old" Oslo CTM3 code)
  MANUAL/    (this manual)
  OSLO/      (Oslo chemistry code)
    DEAD_COLUMN/ (Dust code)
    DUMMIES/    (Dummy routines)
    ROUTINES_NOT_USED/ (Old routines)
  UCI_Q56D/   (original UCI code)
  UCI_Q60A/   (original UCI code)
  tables/     (tables)
    PMEAN/     (to generate annual mean sfcP)
  tmp/       (for compilation)
```

B.2 Checkout

The Oslo CTM3 code is located in a *repository*, and you get it by typing:

```
svn checkout \
  svn+ssh://svn.uio.no/svnroot/osloctm3/ctm3f90 \
  <name of dir to put the code>
```

You can write this on one line in the command window; the backslash allows you to write a command on several lines. The code is now available in your working directory. In the `.svn` directory the original revision files are also available.

If you don't specify the name of directory where the code will be copied to, it will be named `ctm3f90`.

Similarly you can fetch the `utilities` or any other directory from the repository, just swap "`ctm3f90`" with the directory you want. For example, if you only want this manual, use `ctm3f90/MANUAL`.

B.3 Status

SVN can check your working directory files against the original revision of the repository. *It does not check the repository itself!* The status tells you whether the file has changed or not.

```
svn status <file or path>
```

If a file is specified, only that file is checked. If a directory is specified (no specified path or file means current directory) all files in the directory are checked.

The status returns a letter for each file specified:

- ? File does not exist in repository.
- A File is scheduled for addition.
- D File is scheduled for removal.
- C File is in conflict with repository.
- M File is locally modified.

Important

The current version (i.e. the latest repository version) may have changed even though the file status reports the file to be unchanged. Adding an option to the command allows you to see which files that have newer versions in the repository (marked by *):

```
svn status -u <file or path>
```

You can also add a verbose option `-v`.

B.4 Conflicts & resolve

Conflicts occur when you try to update your files, and SVN does not know how to implement your changes into the repository. This must then be *resolved* before you can commit the changes. Resolving can be carried out immediately or be postponed, which is usually the best way.

SVN version 1.4 and older

If you use svn older than version 1.5, you solve a conflict by doing changes to the file and then type:

```
svn resolved <file in conflict>
```

SVN version 1.5 and newer

When getting a conflict for a file, several files are generated, their file names being the original file name + an extension:

- `.mine` Your working copy based on revision XX.
- `.rXX` Revision which your working copy was based on.
- `.rYY` The new file in the repository.

For version 1.5 and newer, the command is `resolve`, and it takes several options. You can decide to use your version

```
svn resolve --accept mine-full \
  <file in conflict>
```

This can also be done by manually correcting the conflicts in the file, followed by

```
svn resolve --accept working \
  <file in conflict>
```

Other possibilities are to accept the repository version (no changes will be committed)

```
svn resolve --accept theirs-full \
  <file in conflict>
```

For resolving conflicts, see Chapter 2 in the SVN book.

B.5 Adding a file

When adding a new file or directory you must first update to the most recent repository version, and then you write

```
svn add <the new file>
```

which schedules the file for the repository. Then you can commit the file:

```
svn commit <the new file>
```

B.6 Deleting a file

If you want to delete a file, simply use the `delete` or `remove` commands, e.g.

```
svn delete <remove-file>
```

which schedules the file for removal, and also removes your local copy. It will be deleted in the repository when you do the commit:

```
svn commit <remove-file>
```

Remember to have the last repository version before deleting files.

You can also delete directories in the same way. In that case, however, the local directory is probably not removed until you commit the changes.

B.7 Committing changes

Not everybody should be allowed to commit changes. A moderator should approve your work before it is committed.

When it has been agreed that your modified files are to be included to the repository, you first need to make sure the file is otherwise updated:

```
svn update
```

Then you can commit the changes, unless there are conflicts;

```
svn commit -m 'msg'
```

where “msg” is a message to tag the changes. Instead of a message you can send in a file where you describe the changes. This is done by `-F <filename>` instead of `-m 'msg'`.

If you only want to commit some of the changed files, use

```
svn commit <files to commit> -m 'msg'
```

B.8 Diff

Diff will give you the differences between your working copy and the revision of the repository it is updated to, i.e. what is located in the `.svn` directory. It does not check the repository!

If you want to compare with other revisions, use the option `-r revision_number`; this will check the repository. The `revision_number` can take several forms, which you should find in the SVN book. The useful revision is usually the latest, and the best solution for this is probably:

```
svn diff -r revision <file>
```

where `revision` may be the wanted revision number, or it may be some date format e.g. `{YYYY-MM-DD}` or `{HH:MM}` (must include parentheses). See the SVN book for more.

B.9 Log

The changes you specify with `-m` when you commit will be stored in a log. You access the log by

```
svn log
```

to get all changes reported, or by

```
svn log <file>
```

to get changes for a specific file.

B.10 Help

You find out more about the SVN commands by typing

```
svn help <command>
```

B.11 Branching

When you start working on a large modification to the Oslo CTM3, it is wise to create a *branch* containing your code. SVN will keep track of your files as before, but it will not affect the trunk – only the branch. Later, when the branch is working well, the branch may be merged into the trunk.

Read the SVN book to find out more on this.

C Technical notes

In this Appendix some technicalities are described, e.g. how the atmosphere is set up.

C.1 AIR mass

The air mass (AIR) is calculated from the pressure, in the routine AIRSET.

Since pressure is force (mg_0) per area, we find the mass of each grid box from the pressure difference Δp between grid box top and bottom, and the grid box area A :

$$m = \frac{\Delta p A}{g_0} \quad (155)$$

This air mass is then the wet air (AIRWET), and dry air is calculated by using the specific humidity (model field Q):

$$m_d = m(1 - Q) \quad (156)$$

When initializing from a restart file, AIR is also initialized from that file.

C.2 Calculation of layer heights

The height of a layer L is calculated by the hypsometric equation

$$\Delta z(L) = \frac{R_d T_v(L)}{g_0} \ln \left(\frac{p(L)}{p(L+1)} \right) \quad (157)$$

where p is the pressure array for the grid box bottom edges, starting at the surface. The model variable is called ZOFLE.

By using specific humidity, the virtual temperature can be calculated:

$$T_v = T(1 - Q) \quad (158)$$

UCI assumes 0.5% mixing ratio, giving $q = 0.005$, and instead of calculating T_v , they calculate the corresponding average gas constant

$$R = R_d(1 - q) + R_v q \approx 288 \quad (159)$$

and use temperature directly. You find this value where they multiply with $29.36 \approx 288/g_0$. This is not done in the Oslo CTM3; we use Q from the meteorological data.

C.3 Calculation of relative humidity

Relative humidity is not available as meteorological field. But it can be calculated from specific humidity (Q). Note that when ECMWF reduced gaussian fields are interpolated, e.g. from T319 to T42, temperature and specific humidity are treated differently. Temperature interpolation takes altitude into account. Thus, in regions of steep mountains, the calculated relative humidity may become unrealistically high. It may also be that the conversion from reduced gaussian grid to regular grid may produce some of the same inconsistencies.

However, the openIFS meteorological data is produced in T159N80L60 resolution, so no conversion to coarser resolution is done.

Specific humidity is defined as

$$Q = \frac{\varrho_v}{\varrho} = \frac{\varrho_v}{\varrho_a + \varrho_v} \quad (160)$$

where ϱ_v is density of water vapor and ϱ_a is density of dry air.

From the equation of state, we have densities expressed by pressure p and temperature T :

$$\varrho_a = \frac{p_a}{R_a T} \quad (161)$$

$$\varrho_v = \frac{p_v}{R_v T} \quad (162)$$

From Eq. (160) we see that

$$\varrho_v(1 - Q) = \varrho_a Q \quad (163)$$

and from Eq. (161-162) we get

$$\frac{R_a}{R_d} p_v (1 - Q) = p_a Q \quad (164)$$

With the usual approximation that $p_a \gg p_v$, so that $p \simeq p_a$, denoting $R_a/R_v = \varepsilon$:

$$p_v = p \frac{Q}{\varepsilon(1 - Q)} \quad (165)$$

For temperature in Kelvin, saturation water vapor pressure ($e_w(T)$) is given by

$$e_w(T) = 611.2 \exp\left(\frac{17.67(T - 273.15)}{T - 29.65}\right) \quad (166)$$

giving relative humidity

$$RH = \frac{p_v}{e_w} \quad (167)$$

Relative humidity with respect to ice is another matter, and requires that you calculate $e_i(T)$ instead of $e_w(T)$.

C.4 How Makefile works

The code is compiled with GNU make; just write `gmake` (or `make`) in the code directory). It reads the *Makefile* and sets up the list of source files and compiles them. All object files are put into the temporary directory *tmp/*. The compilation will be faster by using the option `-j`, e.g. `gmake -j8`.

When you add a file to the code, you need to include some information about it in *Makefile*. This may be a little tricky, so I will go through the steps here.

Adding a new file

Say you add a file to the *OSLO* directory, called *my-file.f90*. Then follow these two steps:

Step 1

Add the file to the source list in *Makefile*: Locate the `OSLO_SRC` variable and add the file name there.

Step 2

Add dependencies; which objects does your file depend on, and which of the existing files depend on your file. These are listed at the bottom of *Makefile*. If your file depend on *cmn_size.f90*, you add

```
$(filter %myfile.o, $(ALL_OBJ)): \
    $(filter %cmn_size.o, $(ALL_OBJ))
```

In the same way you must add `%myfile.o` to the file using your file.

Try to keep the files in alphabetic order in the dependency listing. You only need to list module files and common files, *not* regular subroutine files since those are checked only at the last program linking (but you may still include dependencies if you like).

Adding a new directory

Follow the structure of `OSLO_PATH` and `OSLO_SRC` and create your similar directory `MY_PATH` and list `MY_SRC`.

The path must be added to `ALL_DIRS` and perhaps `INCLUDES`. At the end of the source listing, add `MY_SRC` to `ALL_SRC` (as is done for `OSLO_PATH`).

C.5 DUST map

Input files for the DUST application (Section 15) can be generated with the *map* module written by Charlie Zender. It is located in the directory `/div/amoc/d4-4/oslo-ctm/archive_ctm/ctm_tools/map`. If you want a newer version of *map* you have to contact Zender who develops *map*.

The map-module takes several 1x1 or 0.25 x 0.25 degree files and interpolates them to the desired resolution. Commands to generate datasets are given in the *bds.sh* file in the map-directory.

Having the correct input file, it is important to decide what kind of *erodibility factor* you want to use. The program *bds.F90* contains commands to set the right erodibility factor using the `ncap` command. See Section 15 for more on erodibility factor.

All input data needed for running *map* are available on `/div/amoc/d4-4/oslo-ctm/archive_ctm/input_files/data`.

C.5.1 Libraries needed to run the map module

The map module needs several libraries, also written by Charlie Zender. These libraries are in general non-standard Fortran codes, and are not compiled.

If you want to compile the libraries from scratch (for example on Linux, SGI or HP-UX), you have to compile Charlie's f-module (available on `/div/amoc/d4-4/oslo-ctm/archive_ctm/ctm_tools/libraries/zender_f`), Charlie's c-module (similarly on *zender_c*). In theory: get the files and write *gmake*, in practice, this might cause some pain...

You should have all the compiled library files in one directory, with write access to the directory (you need to write to this directory when running the map module).

After you have the libraries, you need to set the environment variable `MY_LIB_DIR` to be this directory.

All Charlie's programs use the environment variable `NETCDF_INC` and `NETCDF_LIB`, so you might want to set those before you start doing anything else. See Appendix G.1 for paths to netCDF libraries.

D Future work/revisions

During my (Amund) 15-ish years of working with this model, here are some of the changes I think are needed for the Oslo CTM3.

D.1 Optimisation

The parallel region for chemistry spends a lot of time moving data from regular arrays (e.g. `size IPAR,JPAP,LPAR,NPAR`) to private arrays (e.g. `size LPAR,NPAR,IDBLK,JDBLK`).

I think the following should be changed:

- `T` should be converted to `T_LIJ`.
- `GAMA` should be converted to `LIJ`, which could make `GAMAB` unnecessary.
- Diagnostic array `STTTND` should be converted.
- It should be considered to convert all transport arrays also, and do layerwise conversion for horizontal transport. This is a large job and will make the Oslo CTM3 quite different to work with (if you are used to how it is today).

D.2 Dry deposition update

The dry deposition is very crude and should be updated. I have included a first try of the EMEP dry deposition scheme (Section 7.2) and would suggest a proper testing of that.

D.3 New chemistry solver

Ideally, the chemistry routine should cover both troposphere and stratosphere, but this may be a lot of work with current schemes. The best solution, which makes the Oslo CTM3 more flexible (e.g. diagnosing production and loss terms), is to use the kinetical preprocessor (KPP).

Using KPP would make it easier to diagnose chemical production and loss terms.

Tropospheric heterogeneous reactions should be revised, as well as uptake and conversion on tropospheric aerosols.

Sulfur chemistry should be included in the stratosphere. Probably a microphysics scheme for sulfur aerosols should be included.

D.4 Uptake and conversion on aerosols

Uptake of species and conversion on tropospheric aerosols should be revised. I have started this work, it can be found in *aerosols2fastjx.f90*, see Section 12.3.

D.5 J-values

FastJX 7.3 should be implemented. Not very important, though. If not updating to 7.3, OpenMP should be considered included in CLOUD and then tested saved time in T159. Will not save a lot, since it is called only every NMET.

D.6 Aerosol sedimentation

Sedimentation of aerosols should probably be done as separate process, probably using the moments. A first try is given in subroutine *aerosolsettling* in *fallingaerosols.f90*. This will require that gravitational settling in the DUST module will have to be turned off.

D.7 PSC microphysics

I think it should be considered to replace PSC microphysics (Section 11.3) with an even more detailed scheme, without the current assumptions which are somewhat unexplained (unphysical?).

At least, the current 40 size bins makes the code rather slow. Using less bins may be an option; tests have shown that 15 bins may be enough and save some computational time.

D.8 Upper and lower boundary conditions

The upper and lower boundary conditions must be revised: They are taken from the Oslo 2D model, which is outdated and not possible to run. The last year available

is 2011. For upper boundary, a zero flux or other treatment may be considered, otherwise such fields could be generated using e.g. WACCM.

It should be noted that the Oslo 2D model actually uses zero flux conditions, i.e. it could be possible also in Oslo CTM3. But it could lead to a larger drift – may want to have UBC unchanged from year to year. Zero flux is that no tracer leaves UB; we could do chemistry in LPAR or set $\text{mixrat}(\text{LPAR}) = \text{mixrat}(\text{LPAR}-1)$. For long-lived species we could use mixing ratio gradient, but I'm not sure why this would be better than doing chemistry.

D.9 Lightning factors

Note that scaling factors for lightning may not have been produced for all different resolutions and meteorological data.

E Compiler options and optimisation

In *Makefile*, there are three main choices when it comes to optimisation: `OPTS=D` for debug options, `OPTS=O` for O2 optimisation, and `OPTS=A` (denoting more aggressive optimisation) for O3 and a few more additions. O2 is typically judged to be “safe”, whereas O3 may cause small inaccuracies to speed up the code. I have never found O3 to fail, and recommend using `OPTS=A`.

Depending on the machine structure, there are different compilers available, and they have different options.

E.1 Linux

On Linux machines the usual compilers are `intel` and `portland`.

E.1.1 intel – ifort

For more information, see manual pages for `ifort` (man ifort).

Standard options

- `-auto`: Cause all local variables to be allocated on the runtime stack. Default if OpenMP.
- `-fpp`: Enable use of C preprocessor really only needed for *.F90* files and not *.f90* files, but doesn't harm compilation of *.f* files.
- `-ftz`: Set abnormally low values to zero; i.e. values below 10^{-34} will be zero if `real*4` is used.
- `-mcmodel=large`: Allow for large executable file as we will get with many components and high resolution (medium can be set to `large`).
- `-shared-intel`: Libraries provided by intel are linked dynamically (old intel versions: `i-dynamic`).

Debug options

- `-mp`: Maintain floating point precision. This will reduce optimisations!

- **-check bounds**: Check array bounds.
- **-check uninit**: Check whether variables are used without being initialised first.
- **-traceback**: Should trace back the error to a specific line in the code.
- **-openmp**: Enable OpenMP.

Optimizing options

- **-inline-forceinline**: Inline code (see O2 option).
- **-O2**: Including global code scheduling⁵, software pipelining⁶, predication, and speculation⁷. It also enables inlining⁸ and removes unreferenced variables.
- **-openmp**: Enable OpenMP.
- **-mp1**: As **-mp**, it tries to maintain floating point precision, but disables fewer optimisations than **-mp** (see below).

Aggressive optimizing options

As for Optimizing options, but instead of **-O2**, use

- **-O3**: Enables **-O2** optimisations plus more aggressive optimisations, such as prefetching⁹, scalar replacement¹⁰, and loop transformations. Enables optimisations for maximum speed, but does not guarantee higher performance unless loop and memory access transformations take place.

In addition use

- **-fno-alias**: Specifies that aliasing should not be assumed in the program.
- **-fomit-frame-pointer**: Disables use of EBP as a general purpose register so it can be used as a stack frame pointer.

E.1.2 portland – pgf90

For more information, see manual pages for **pgf90** (**man pgf90** or **pgf90 -help**).

Standard options

- **-mmodel=medium**: Allow for large executable file. Necessary to run the Oslo CTM3.

Debug options

- **-Mbounds**: Check array bounds.
- **-g**: Generate symbolic debug information.

Optimizing options

- **-O2**: Including global code scheduling.
- **-mp**: Enable OpenMP.
- **-Minline**: Pass options to the function inliner.
- **-Mprefetch**: Pass options to the function inliner.

Aggressive optimizing options

As for Optimizing options, but instead of **-O2**, use

- **-O3**: Enables **-O2** optimisations plus more aggressive optimisations.

⁵Schedule instruction so that hardware is effectively used

⁶Makes the processor work all the time, avoids waiting

⁷E.g. guesses results of if-tests and starts calculations in advance

⁸Include subroutines directly into code

⁹Grabs code and starts calculating instead of waiting for the calculation to arrive

¹⁰Checks if any calculation can be replaced by constants

- **-mp**: Enable OpenMP.
- **-Minline=reshape**: Pass options to the function inliner. Also reshape arrays that would hinder normal inlining.
- **-Mprefetch**: Add (don't add) prefetch instructions for those processors that support them.
- **-Munroll**: Unroll loops.

F HPC

You will probably use a high performance computing (HPC) facility to run the model. These usually require that you submit a simulation to a queue system, using a job script.

Some smaller systems may not have queues, but use the traditional **nohup** command. Queue systems usually also have a possibility to run jobs *interactively*, meaning that you can log on to a computer and run the model in your terminal window. This is the typical choice for testing your program.

You will have to find a suitable computer or cluster to run the model.

Some computing clusters use the slurm queue system. An example can be found in the job file example *c3run.job* in your working directory, or the example given in Table 29 and 30.

Basically, the script consists of four steps: First is the setting of number of CPUs and memory usage, second copying and linking to work (scratch) directory, then running the model and copying the results to somewhere else.

Directory names can be modified, as well as the copying and linking statements.

It is vital to set the stack size properties, also when you do not use a queue system.

F.0.3 slurm interactively

To run the model interactively, use **qlogin**. You will also need to specify the account, CPUs etc (see top of Table 29).

You need to be a bit careful when setting the memory per CPU; the total (number of CPUs times memory per CPU) should not exceed what is available on a node.

It may be that the cluster also have some nodes with more memory than this, possibly defined by an option such as **hugemem** (see top of Table 29).

To have an idea on the total memory required to run the model, use the UNIX command **size**:

```
size osloctm3
```

and look at the number **bss**, which for T42L60 with tropospheric and stratospheric chemistry is typically between 5 GB and 9 GB depending on which modules you include.

Table 29: Job script for USIT HPC, part 1.

```
#!/bin/bash
# Job name:
#SBATCH --job-name=testscript
# Project:
#SBATCH --account=account_name
# Wall clock limit:
#SBATCH --time=1:0:0
# Max memory usage:
#SBATCH --mem-per-cpu=2000M
# Possibly use hugemem nodes
####SBATCH --partition=hugemem
# Number of cores:
#SBATCH --ntasks-per-node=8
# Number of nodes:
#SBATCH --nodes=1
# Work disk space
#SBATCH --tmp=60G
# Set up job environment
source /site/bin/jobsetup
# -----
# No need to change this section

# Must set large stack size (unlimited)
ulimit -s unlimited
# Set ulimit also to unlimited
ulimit unlimited
# Print out information about ulimit
ulimit -a

# allocate specified memory to each thread
export THREAD_STACKSIZE=100m
# ifort: KMP_STACKSIZE
export KMP_STACKSIZE=$THREAD_STACKSIZE

# number of OpenMP threads (number of CPUs)
export OMP_NUM_THREADS= \
    $SLURM_NTASKS_PER_NODE
```

While running your program interactively, you can also use the command `top` to see the virtual memory used by your program.

Interactively 8 CPUs

```
qlogin --account=ACCOUNT_NAME \
    --ntasks-per-node=8 \
    --mem-per-cpu=2000M
    --nodes=1
```

If your specified amount of memory is too low, or the defined stack size is too low, the program may stop. The latter will usually only produce a segmentation fault, while the first may produce better info.

Given that the program stops with a segmentation fault, try setting:

```
ulimit -s unlimited
```

Table 30: Job script for USIT HPC, part 2.

```
# the PID number (if you want it)
export PID='date +%d%m%y'.'$$'

# -----
# Do changes here

# Model dir
export MODELDIR=$HOME/WHERE_THE_MODEL_IS

# Scenario name (use e.g. job name)
export SCEN=$SLURM_JOB_NAME

# Result directory at $HOME
export RESULTDIR=$HOME/DONE.$SCEN

# Copy or link files to work directory:
cp $MODELDIR/myprogram $SCRATCH/

# Go to work directory
cd $SCRATCH

# Run command (using $SCEN)
./myprogram > results.$SCEN

# Make the result directory
mkdir $RESULTDIR

# Copy files to result directory
cp results* $RESULTDIR/

# Done
```

If that does not help, try to increase the thread stack size:

```
export THREAD_STACKSIZE=300m
export KMP_STACKSIZE=$THREAD_STACKSIZE
```

These should be set in job scripts, but may be too low for some applications.

Remember the UNIX command `size` to get an idea on the total memory required.

F.0.4 Checking your run

You can check your run using the command `squeue`. If you want more info than standard output, you can e.g. use (put everything on one line):

```
squeue -o '%.8i %.16j %.8u %.1t %.10M %.4C %.5D
          %R' -S '-t' -u USER
```

where `USER` is your user name.

To check end time (put everything on one line):

```
squeue -o '%.8i %.16j %.8u %.9a %.1t %.19e %.10M %.4C %.5D
          %.7m %R' -S '-t' -u USER
```

To check time and time left (put everything on one line):

```
squeue -o '%.8i %.12j %.8u %.7a %.1t %.10M %.10L %.3C %.3D'
        %R' -S '-e' -u USER
```

G External libraries

So far the only external libraries needed to run the Oslo CTM3 is netCDF.

G.1 netCDF

To run the model, you need the netCDF libraries, and their path should be exported as environment variables `NETCDF_INC` and `NETCDF_LIB`. This is done in *Makefile*, and the paths are given here for different machines.

Abel

Use `module load netcdf.intel` or similar for other compilers. This sets environment variables used by *Makefile*.

G.2 HDF

No need for HDF, but if you are considering it, here is a note: Using both HDF and netCDF may not work unless they are compiled with the same of compiler version.

H Meteorological data

So far the Oslo CTM3 only reads ECMWF data produced at UiO, but can be set up to use data from any GCM, as long as the required meteorological fields are available.

Until 2015, the meteorological data were produced with the Integrated Forecast System (IFS) model at the ECMWF computing facilities. During 2015, the openIFS model was installed at the UiO computing facility Abel. This allowed production of more years of data.

The openIFS data are available in the old UiO binary format, and also in netcdf4. Standard read-in is netcdf4.

At CICERO, the data are stored at `/div/pdo/metdata/`, and as the catalogue names indicate, there are data from different cycles of IFS, and also data from the openIFS model.

Note that the data must be copied to the computer system where the Oslo CTM3 is to be run. At CICERO we have put most of what is needed at `/div/amoc/d4-4/oslo-ctm/` and `/work/projects/cicero/ctm_input`.

H.1 ECMWF meteorological data

The IFS/openIFS data are 36-hour forecasts, with 12 hours spinup, starting from reanalyses fields at 12 UTC the day before. Since cycle 36r1, the reanalyses have been from ERA-Interim, but before that the IFS model was started from operational analyses.

Table 31: Resolutions available from the ECMWF, taken from <http://www.ecmwf.int/>

| Spectral | Grid | Degrees | IPAR | JPAR |
|----------|------|---------|------|------|
| T42 | N32 | 2.8125 | 128 | 64 |
| T63 | N48 | 1.875 | 192 | 96 |
| T106 | N80 | 1.125 | 320 | 160 |
| T159 | N80 | 1.125 | 320 | 160 |
| T319 | N160 | 0.5625 | 640 | 320 |
| T511 | N256 | 0.351 | 1024 | 512 |
| T799 | N400 | 0.225 | 1600 | 800 |
| T1023 | N512 | 0.176 | 2048 | 1024 |

Typical ECMWF horizontal resolutions are listed in Table 31. We use T159/N80 in openIFS, while the older IFS cycle 36r1 used T319/N160. The IFS and openIFS models are usually run in Gaussian reduced grids, but at least the IFS model has previously been used to put out data on regular grids.

Conversion from reduced Gaussian grid to regular Gaussian grid is done with the GRIB API, either at the ECMWF or locally.

H.1.1 File format

Until 2015, the meteorological data were provided in a binary little-endian format, the UiO binary format.

Since late 2015, the meteorological data are available in netCDF4 format, which is now the standard read-in for Oslo CTM3.

You define which format to use by the `metTYPE` in *LxxCTM.inp*:

- **ECMWF_oIFSnc4**: OpenIFS generated in netCDF4 format.
- **ECMWF_oIFS**: OpenIFS generated in UiO binary format.
- **ECMWF_IFS**: IFS data generated in UiO binary format.

However, to use the UiO binary format you need to use a different read-in, which can be found in *met-data_ecmwf_uioformat.f90*. The Oslo CTM3 should tell you if that is the case.

UiO binary format

The UiO binary format provides data in 3 files per day:

- Files *EC*.b01*: Spectral data.
- Files *EC*.b02*: 3D data on gaussian grid.
- Files *EC*.b03*: Surface (2D) data.

All data for one meteorological time step is written before the next time step is written, allowing a sequential read. This is rather quick, since when continuing read-in for a time step always continues where you left off in the previous time step. Spectral data are converted using a fast Fourier transform.

netCDF4 format

In the netCDF4 format, all meteorological fields are given on one file per meteorological time step. This means that there are 8 files per day; 2790 files per year. They have

therefore been grouped in directories for each month. This is the quickest way to access all data for a time step, so the netCDF will not have to locate a part of a 3D or 4D array, but can access the fields almost sequential.

H.1.2 Available fields

The meteorological fields, including their names, details and ID numbers (the UiO format IDs) are given in Table 35–37 (tables located after references). The netCDF4 files also contain info about the grid, which are also listed in the tables.

IFS and openIFS generally use the local table 2 version 128 for naming and numbering of output variables. The UiO format IDs generally follow this table, with the exception of the extra fields put out.

ECMWF uses GRIB output format, so their result files have to be converted to our format. This is done locally at CICERO/UiO, and currently involves creating UiO binary format files, which are then converted to netCDF4. A short description on how to do this is described in Appendix H.1.3.

H.1.3 Producing openIFS data

At Abel, the openIFS model was set up in 2015. As the IFS model before it, it includes a special branch that diagnoses the convective mass fluxes and 3D precipitation fluxes (convective and large scale).

To run the openIFS model, it must be compiled, and at Abel it can be loaded using module:

```
module load openifs
```

In the *openifs/38r1v04/* directory (or *openifs/40r1v1/* for cycle 40r1), located in */cluster/software/VERSIONS/*, you find the subdirectory *osloctm*. In principle this should be copied to your own suitable directory, but in my opinion the files should be slightly modified. Such modified files can be found in the repository directory *utilities/generateOpenIFS*.

There are four job scripts that you will use, and one input file:

- *getEIdata.job*
- *runInterpolation.job*
- *runOpenIFS.job*
- *runECgrib2CTM.job*
- *initrun*

The scripts should be run separately, although it is possible to let one start the next. That has been tested and may cause problems.

In *initrun*, you define the resolution and date to retrieve. It should look like this for T159L60N80 resolution:

```
# Experiment id (has to stay the same from
# interpolation to running openIFS.
EXPVER=b0z5
# Resolution
```

```
RESOL=159
# Number of vertical levels
LEVELS=60
# reduced GG to regular GG
NGG=80
# for openIFS 1_2 if higher resolution is used
GRID_TYPE="1_2"
```

```
# start date YYYYMMDD
SDATE=20150801
# end date YYYYMMDD
EDATE=20150831
# TIME is given as a list of times separated
# by / i.e. 00/12
TIME=12
# TIMESTEP timestep to run openIFS
TIMESTEP=1200.0
# FLENGTH is the FORECAST LENGTH (hours) to
# run openIFS
FLENGTH=36
```

EXPVER is experiment version you may alter, however, it has to stay the same from interpolation to running the OpenIFS.

TIME is the start hour of the run, which is noon. If you specify other values also, you will get more data. This is not necessary.

To use coarser resolution such as RESOL=42, you need to set GRID_TYPE=_2.

The job scripts needs an environment variable WORKDIR, which on Abel is your work directory. These are set up when you load openIFS using module.

Retrieve analyses from ECMWF

To retrieve restart fields for openIFS, you must have a registered account at ECMWF, see *software.ecmwf.int/wiki/display/OIFS/* for more on this.

The *getEIdata.job* will put retrieved reanalysis fields in the directory *\$WORKDIR/EI/*. Retrieving one month of data usually takes less than one hour. It is wise to download several months of data before doing the next steps.

Important

ECMWF wants you to download *no more* than one month of data in each job.

Interpolate to specified resolution

I have set up *runInterpolation.job* to use 12 CPUs on one node, since I found it most effective (less queue, still fairly fast).

Interpolated fields will be located in the directory *\$WORKDIR/\$RESOL/*.

Interpolating one month of data usually takes less than 15 minutes. I suggest running at least 3 months at a time.

Run the openIFS

I have set up *runOpenIFS.job* to use 16 CPUs on one node, since I found it most effective. Running one month usually takes about 2 hours. 32 CPUs on several nodes is usually not much faster; it is very often slower.

Output will be located in the directory

`$WORKDIR/$RESOL/`.

Convert to UiO binary format

`runECgrib2CTM.job` runs on 1 CPU, and takes a bit of time. It reads GRIB files and converts to UiO binary format.

Output will be located in the directory `$WORKDIR/OSLOCTM/$RESOL`.

Processing one month usually takes about 2–3 hours.

Note that the file day number changes from openIFS to CTM fields, which is because the openIFS was started at noon and we only use data for the next day.

Convert to netCDF4

In the repository utilities, there is a fortran program available which converts UiO binary format to netCDF4. The program is available at `utilities/fortran/ec2netcdf4/`, and at the top of the source code you find info on how to compile it.

You must specify where the UiO binary files are. After compiling the program, you run it using

```
ec2netcdf4 YYYY
```

where YYYY is the year to process. Output data will be placed in the directory where you run the program.

H.1.4 Producing IFS data

Since 2015 we started using the openIFS model for producing meteorological data, but here is a very short description of how IFS retrieval worked.

The IFS model is run through web interface at the ECMWF, where you select the wanted resolution.

After that the archived data are retrieved in the same or lower resolution (it is interpolated at ECMWF). Note that the native resolution usually is *reduced* Gaussian, and we need to specify we need *regular* Gaussian data. This is a user choice in the retrieval of data from the MARS archive at ECMWF.

The files retrieved from ECMWF are on GRIB format, from which the UiO binary format files are retrieved locally at UiO.

H.2 Meteorological fields in the Oslo CTM3

The Oslo CTM3 puts the meteorological data into arrays, where some are used directly, and others are converted to the suitable units. As already explained, the variable names are listed and described in Table 35–37 (tables located after references).

Some meteorological fields are described more closely here.

H.2.1 Convective mass flux

The updraft mass flux (CWETE) and downdraft mass flux (CWETD, which is negative downwards) is given on *half-levels*, meaning they are values valid at the *bottom of each grid box*.

Their original units are accumulated $\text{kg}/(\text{m}^2\text{s})$, and since the flux up or down at the surface it is always zero, the *first level stored is for layer 2*.

Conversion to kg/s is done by dividing by the time span (3 hours for ECMWF IFS and openIFS) and multiplying with grid box area.

More special is the entrainment into updrafts CENTU and into downdrafts CENTD. These are built from detrainment rates, which are given as accumulated $\text{kg}/(\text{m}^2\text{s})$ per grid height, so the units are accumulated $[\text{kg}/(\text{m}^3\text{s})]$. Detrainment rates are given for *full-levels*, i.e. grid center values.

To convert to detrainment fluxes, these rates are multiplied with grid height and area and divided by the time span. Entrainment (E) is build from the mass flux (F) in at bottom and out of top and detrainment (D) by considering incoming versus outgoing air:

$$F(L) + E(L) = F(L+1) + D(L) \quad (168)$$

Another way to look at this is similarly to the IFS documentation

$$\frac{dF}{dz} dz = E(L) - D(L) \quad (169)$$

which gives the same result

$$F(L+1) - F(L) = E(L) - D(L) \quad (170)$$

Equation (168) applies for downdrafts as well, since the downdraft mass fluxes are negative (total mass in: $-F(L+1) + E$, total mass out: $-F(L) - D$).

H.3 GCM meteorological data

If you want to set up the model to use meteorological data from a GCM, you need the correct hybrid coordinates, and you need to make a new routine reading the data. Note that if the GCM puts out spectral data, the Oslo CTM3 routines for converting to gridded data may not be suitable, so it may be best to use gridded data directly.

Also note that for the boundary layer height BLH, the retrieval of the next time step value (BLH_NEXT) may be difficult if the data are structured in a bad way (but not impossible, of course).

H.3.1 Read-in routine

There is no read-in available for other meteorological data, so you have to make your own. Use the ECMWF read-in as starting point.

I Trouble shooting

When you log on to the computers, you may experience a few problems. Do not hesitate to ask the experienced Oslo CTM3 users about this, they have probably been there!

One of the first problem you will run into is the compiling. You choose the compiler in *Makefile*, and it is typically intel.

The compilers may not be loaded by default, you may need to load them manually. Ask the experienced users or see the user manual for the computing facility.

The next problem is probably that the model crashes, so you should look up Appendix F for environment variables you need to set; `OMP_NUM_THREADS` and `KMP_STACKSIZE` (for intel). And you also need to set

```
ulimit -s unlimited
```

If the program says “OpenMP cannot create thread”, it is often a stack size problem, but it can also be problems with arrays not declared correctly (e.g. in arguments etc.). Look in parallel regions first.

Also, the program may just say “Segmentation fault” if you have set the `KMP_STACKSIZE` too low.

-O3 floating point exception

If you compile a loop where one index of the loop is zero (set by parameter), the compiling may fail in the Optimizer loop nesting. Can usually be solved by better programming on the loop.

To stop when array is out of bounds

You force the program to stop at array out of bounds by setting the environment variable

```
export F90_BOUNDS_CHECK_ABORT=YES
```

Strange things happen

If suddenly very strange messages occur when compiling, there may have been e.g. updates to compilers. Clear the compilation (`gmake clean`) and compile all from start.

J Chemical reactions

Reactions taken into account in the Oslo CTM3 are listed here, separated into photolytic reactions, bi-molecular reactions, tri-molecular reactions, and heterogeneous reactions.

Listed are the JPL (Sander et al., 2006) reaction numbers, that consist of a letter followed by number (e.g. A1), and the IUPAC (Atkinson et al., 2010) numbers which use more letters to describe the reaction. The numbering should be evident once you look at JPL/IUPAC.

If reaction data are provided by both JPL and IUPAC, the number in *italics* is not used. In the tables below, the JPL/IUPAC values are listed as 'Reference' or 'Ref.'.

J.1 Photolytic reactions

Tropospheric chemistry module

| Reaction | Reference |
|---|-------------|
| Ox | |
| $\text{O}_3 + h\nu \longrightarrow \text{O}_2 + \text{O}(^3\text{P})$ | A1/ |
| $\text{O}_3 + h\nu \longrightarrow \text{O}_2 + \text{O}(^1\text{D})$ | A2/ |
| HOx | |
| $\text{H}_2\text{O}_2 + h\nu \longrightarrow 2\text{OH}$ | B3/ |
| NOx | |
| $\text{NO}_2 + h\nu \longrightarrow \text{NO} + \text{O}(^3\text{P})$ | C1/PNOx4 |
| $\text{NO}_3 + h\nu \longrightarrow \text{NO}_2 + \text{O}(^3\text{P})$ | C2a/PNOx5 |
| $\text{N}_2\text{O}_5 + h\nu \longrightarrow \text{NO}_2 + \text{NO}_3$ | C5/PNOx7 |
| $\text{HNO}_3 + h\nu \longrightarrow \text{NO}_2 + \text{OH}$ | C7/PNOx2 |
| $\text{HO}_2\text{NO}_2 + h\nu \longrightarrow \text{NO}_2 + \text{HO}_2$ | C8a+b/PNOx3 |
| Organic | |
| $\text{CH}_2\text{O} + h\nu \longrightarrow \text{H} + \text{HCO}$ | D1/P1 |
| $\text{CH}_2\text{O} + h\nu \longrightarrow \text{H}_2 + \text{CO}$ | D1/P1 |
| $\text{CH}_3\text{CHO} + h\nu \longrightarrow \text{CHO} + \text{CH}_3$ | D2/P3 |
| $\text{CH}_3\text{O}_2\text{H} + h\nu \longrightarrow \text{OH} + \text{CH}_3\text{O}$ | D7/P12 |
| $\text{CH}_3\text{COCH}_2\text{CH}_3 + h\nu \longrightarrow$ $\text{CH}_3\text{CO} + \text{C}_2\text{H}_5\text{O}_2$ | /P8 |
| $\text{CH}_3\text{COCOCH}_3 + h\nu \longrightarrow 2 \text{CH}_3\text{CO}$ | use D18/P6 |
| $\text{HCOHCO} + h\nu \longrightarrow \text{CO} + \text{CH}_2\text{O}$ | D17/P4 |
| $\text{CH}_3\text{COHCO} + h\nu \longrightarrow$ $\text{CO} + \text{CH}_3\text{CHO}$ | D18/P6 |
| $\text{CH}_3\text{COCH}_3 + h\nu \longrightarrow$ $\text{CH}_3\text{CO} + \text{CH}_3$ | /0.7P8 |

Stratospheric chemistry module

| Reaction | Reference |
|--|-----------|
| Ox | |
| $\text{O}_3 + h\nu \longrightarrow \text{O}_2 + \text{O}(^3\text{P})$ | A2/POx1 |
| $\text{O}_3 + h\nu \longrightarrow \text{O}_2 + \text{O}(^1\text{D})$ | A2/POx1 |
| $\text{O}_2 + h\nu \longrightarrow 2 \text{O}(^3\text{P})$ | A1/POx2 |
| HOx | |
| $\text{H}_2\text{O} + h\nu \longrightarrow \text{OH} + \text{H}$ | B2/PHOx1 |
| $\text{H}_2\text{O}_2 + h\nu \longrightarrow 2\text{OH}$ | B3/PHOx2 |
| NOx | |
| $\text{NO} + h\nu \longrightarrow \text{N} + \text{O}$ | N/A |
| $\text{NO}_2 + h\nu \longrightarrow \text{NO} + \text{O}(^3\text{P})$ | C1/PNOx4 |
| $\text{NO}_3 + h\nu \longrightarrow \text{NO}_2 + \text{O}(^3\text{P})$ | C2a/PNOx5 |
| $\text{NO}_3 + h\nu \longrightarrow \text{NO} + \text{O}_2$ | C2b/PNOx5 |
| $\text{N}_2\text{O} + h\nu \longrightarrow \text{N}_2 + \text{O}(^1\text{D})$ | C3/PNOx6 |
| $\text{N}_2\text{O}_5 + h\nu \longrightarrow \text{NO}_2 + \text{NO}_3$ | C5/PNOx7 |
| $\text{HNO}_3 + h\nu \longrightarrow \text{NO}_2 + \text{OH}$ | C7/PNOx2 |
| $\text{HO}_2\text{NO}_2 + h\nu \longrightarrow \text{NO}_2 + \text{HO}_2$ | C8a/PNOx3 |
| $\text{HO}_2\text{NO}_2 + h\nu \longrightarrow \text{NO}_3 + \text{OH}$ | C8b/PNOx3 |
| Organic | |
| $\text{CH}_2\text{O} + h\nu \longrightarrow \text{H} + \text{HCO}$ | D1/P1 |
| $\text{CH}_2\text{O} + h\nu \longrightarrow \text{H}_2 + \text{CO}$ | D1/P1 |
| $\text{CH}_3\text{O}_2\text{H} + h\nu \longrightarrow \text{CH}_3\text{O} + \text{OH}$ | N/A |

| | | | |
|---|-----------|--|----------------|
| ClOx | | | |
| $\text{Cl}_2 + h\nu \longrightarrow \text{Cl} + \text{Cl}$ | F1/PC111 | $\text{OH} + \text{C}_3\text{H}_8 \longrightarrow$ | D22/HOx_VOC6/ |
| $\text{ClO} + h\nu \longrightarrow \text{Cl} + \text{O}(^3P)$ | F2/ | $\text{C}_3\text{H}_7\text{O}_2 + \text{H}_2\text{O}$ | R4048 |
| $\text{OCIO} + h\nu \longrightarrow \text{O}(^3P) + \text{ClO}$ | F4/PC13 | $\text{OH} + \text{C}_4\text{H}_{10} \longrightarrow$ | /HOx_VOC7/ |
| $\text{Cl}_2\text{O}_2 + h\nu \longrightarrow \text{ClOO} + \text{Cl}$ | F7/PC15 | $\text{C}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$ | R4010 |
| $\text{OHCl} + h\nu \longrightarrow \text{OH} + \text{Cl}$ | F14a/PC12 | $\text{OH} + \text{C}_6\text{H}_{14} \longrightarrow$ | NA/R4011 |
| $\text{ClONO}_2 + h\nu \longrightarrow \text{Cl} + \text{NO}_3$ | F18/PC110 | $\text{C}_6\text{H}_{13}\text{O}_2 + \text{H}_2\text{O}$ | NA/R4012 |
| $\text{CF}_2\text{Cl}_2 \text{ (CFC12)} + h\nu \longrightarrow \text{Clx}$ | /PC115 | $\text{OH} + \text{m-Xylene} \longrightarrow 0.6\text{AR1}$ | HOx_VOC8/R4020 |
| $\text{CFCl}_3 \text{ (CFC11)} + h\nu \longrightarrow \text{Clx}$ | PC116 | $\text{OH} + \text{Isoprene} \longrightarrow \text{ISOR1}$ | D14/R4013 |
| $\text{CHF}_2\text{Cl (HCFC22)} + h\nu \longrightarrow \text{Clx}$ | /PC114 | $\text{OH} + \text{HCHO} \longrightarrow \text{CHO} + \text{H}_2\text{O}$ | D35/R2122 |
| $\text{CH}_3\text{Cl} + h\nu \longrightarrow \text{Clx}$ | /PC112 | $\text{CH}_3\text{O}_2 + \text{HO}_2 \longrightarrow$ | |
| $\text{CH}_3\text{CCl}_3 + h\nu \longrightarrow \text{Clx}$ | /PC120 | $\text{CH}_3\text{O}_2\text{H} + \text{O}_2$ | |
| $\text{CF}_3\text{CHCl}_2 \text{ (HCFC123)} + h\nu \longrightarrow \text{Clx}$ | F42/PC122 | $\text{CHO} + \text{O}_2 \longrightarrow \text{HO}_2 + \text{CO}$ | D44/RCHOM |
| $\text{CF}_2\text{ClCFCl}_2 \text{ (CFC113)} + h\nu \longrightarrow \text{Clx}$ | /PC123 | $\text{CH}_3\text{O} + \text{O}_2 \longrightarrow \text{HO}_2 + \text{HCHO}$ | D46/RCH3OM |
| $\text{CF}_2\text{ClCF}_2\text{Cl (CFC114)} + h\nu \longrightarrow \text{Clx}$ | /PC124 | $\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \longrightarrow$ | D50/R2222 |
| $\text{CF}_3\text{CF}_2\text{Cl (CFC115)} + h\nu \longrightarrow \text{Clx}$ | /PC125 | $0.4(2\text{CH}_3\text{O} + \text{O}_2)$ | |
| $\text{CH}_3\text{CFCl}_2 \text{ (HCFC141b)} + h\nu \longrightarrow \text{Clx}$ | F45/PC119 | $+ 0.6\text{HCHO}$ | |
| $\text{CH}_3\text{CF}_2\text{Cl (HCFC142b)} + h\nu \longrightarrow \text{Clx}$ | F46/PC118 | $\text{OH} + \text{CH}_3\text{O}_2\text{H} \longrightarrow$ | D16/R4016A |
| BrOx | | $\text{CH}_3\text{O}_2 + \text{H}_2\text{O}$ | |
| $\text{Br}_2 + h\nu \longrightarrow \text{Br} + \text{Br}$ | G1/PBr9 | $\text{OH} + \text{CH}_3\text{O}_2\text{H} \longrightarrow$ | D16/R4016B |
| $\text{HBr} + h\nu \longrightarrow \text{H} + \text{Br}$ | G2/PBr1 | $\text{HCHO} + \text{OH} + \text{H}_2\text{O}$ | |
| $\text{BrO} + h\nu \longrightarrow \text{Br} + \text{O}$ | G3/PBr3 | $\text{OH} + \text{AR2} \longrightarrow \text{AR3}$ | NA/R4030 |
| $\text{OHBr} + h\nu \longrightarrow \text{OH} + \text{Br}$ | G6/PBr2 | $\text{OH} + \text{CH}_3\text{COCH}_2\text{CH}_3 \longrightarrow$ | HOx_VOC20/ |
| $\text{BrONO}_2 + h\nu \longrightarrow \text{BrO} + \text{NO}_2$ | G9/PBr7 | $\text{CH}_3\text{COCH}(\text{O}_2)\text{CH}_3$ | R4019 |
| $\text{BrCl} + h\nu \longrightarrow \text{Br} + \text{Cl}$ | G10/PBr8 | $\text{OH} + \text{ISOK} \longrightarrow$ | HOx_VOC21/ |
| $\text{CH}_3\text{Br} + h\nu \longrightarrow \text{Bry}$ | G12/PBr10 | ISOR2 | R4033 |
| $\text{CF}_2\text{ClBr (Halon-1211)} + h\nu \longrightarrow \text{Bry}$ | G25/PBr12 | $\text{OH} + \text{HCOHCO} \longrightarrow$ | HOx_VOC16/ |
| $\text{CF}_3\text{Br (Halon-1301)} + h\nu \longrightarrow \text{Bry}$ | G26/PBr11 | $\text{fa}_{45}(\text{CHO} + \text{CO})$ | R4035A |
| | | $+ \text{fb}_{45}(\text{CH}_3\text{CO})$ | R4035B |
| | | $+ \text{fc}_{45}(2\text{CO} + \text{HO}_2)$ | R4035B |
| | | $\text{OH} + \text{RCOHCO} \longrightarrow$ | HOx_VOC18/ |
| | | $\text{CH}_3\text{CO} + \text{CO}$ | R4036 |
| | | $\text{OH} + \text{CH}_3\text{COCH}_3 \longrightarrow$ | HOx_VOC19/ |
| | | $\text{H}_2\text{O} + \text{CH}_3\text{COCH}_2$ | R4050 |
| | | $\text{O}_3\text{CH}_3\text{COCH}_2(\text{O}_2)$ | |
| | | $\text{OH} + \text{CH}_3\text{CHO} \longrightarrow$ | HOx_VOC12/ |
| | | $\text{CH}_3\text{CO} + \text{H}_2\text{O}$ | R4014 |
| | | $\text{OH} + \text{PAN} \longrightarrow \text{HCHO} + \text{NO}_2$ | HOx_VOC44 |
| | | $+ \text{CO}_2 + \text{H}_2\text{O}$ | R4005 |
| | | $\text{NO} + \text{CH}_3\text{O}_2 \longrightarrow$ | D51/ |
| | | $\text{fa}_{48}(\text{NO}_2 + \text{CH}_3\text{O})$ | R4322 |
| | | $\text{NO} + \text{C}_2\text{H}_5\text{O}_2 \longrightarrow \text{fa}_{49}(\text{NO}_2$ | D57/ROO_2/ |
| | | $+ (1-\text{fb}_{49})(\text{HCHO} + \text{CH}_3)$ | R4323 |
| | | $+ \text{fb}_{49}(\text{HO}_2 + \text{CH}_3\text{CHO}))$ | |
| | | $\text{NO} + \text{C}_3\text{H}_7\text{O}_2 \longrightarrow \text{fa}_{50}(\text{NO}_2$ | ROO_4/ |
| | | $+ (1-\text{fb}_{50})(\text{CH}_3\text{CHO} + \text{CH}_3\text{O}_2)$ | R4349 |
| | | $+ \text{fb}_{50}(\text{HO}_2 + \text{CH}_3\text{COCH}_3))$ | use ROO_4/ |
| | | $\text{NO} + \text{C}_4\text{H}_9\text{O}_2 \longrightarrow \text{fa}_{51}(\text{NO}_2$ | R4324 |
| | | $+ (1-\text{fb}_{51})(\text{CH}_3\text{CHO}$ | |
| | | $+ \text{C}_2\text{H}_5\text{O}_2)$ | |
| | | $+ \text{fb}_{51}(\text{HO}_2$ | |
| | | $+ \text{CH}_3\text{COCH}_2\text{CH}_3))$ | use ROO_4/ |
| | | $\text{NO} + \text{C}_6\text{H}_{13}\text{O}_2 \longrightarrow \text{fa}_{52}(\text{NO}_2$ | R4325 |
| | | $+ \text{C}_4\text{H}_9\text{O}_2 + \text{CH}_3\text{CHO})$ | use D51/ |
| | | $\text{NO} + \text{AR1} \longrightarrow \text{NO}_2 + \text{HO}_2$ | R4329 |
| | | $+ \text{AR2} + \text{RCOHCO}$ | use D51/ |
| | | $\text{NO} + \text{AR3} \longrightarrow \text{NO}_2 + \text{HO}_2$ | R4331 |
| | | $+ \text{HCOHCO} + \text{RCOHCO}$ | use D51/ |
| | | $\text{NO} + \text{ISOR1} \longrightarrow \text{fa}_{55}(\text{NO}_2 + \text{HO}_2$ | R4332 |
| | | $+ \text{ISOK} + \text{HCHO})$ | use D51/ |
| | | $1.5\text{NO} + \text{ISOR2} \longrightarrow$ | R4334 |
| | | $1.5\text{NO}_2 + 0.67\text{HO}_2$ | |
| | | $+ 0.43\text{HCHO} + 0.67\text{RCOHCO}$ | |
| | | $+ 0.33\text{CH}_3\text{CO} + 0.33\text{CH}_3\text{CHO}$ | use D51/ |
| | | $\text{NO} + \text{CH}_3\text{COCH}(\text{O}_2)\text{CH}_3 \longrightarrow$ | R4327 |
| | | $\text{fa}_{57}(\text{NO}_2 + \text{HO}_2$ | |
| | | $+ \text{CH}_3\text{COCOCCH}_3)$ | |
| | | $\text{NO} + \text{CH}_3\text{COCH}_2(\text{O}_2) \longrightarrow$ | use D51/ |
| | | $\text{NO}_2 + \text{HO}_2 + \text{CH}_3\text{COCHO}$ | R4351 |
| | | $\text{NO} + \text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} \longrightarrow$ | use D51/ |
| | | $\text{NO}_2 + \text{HCHO}$ | R4328 |
| | | $+ \text{CH}_3\text{CHO} + \text{HO}_2$ | |
| | | $\text{NO}_3 + \text{CH}_3\text{CHO} \longrightarrow$ | D41/ |
| | | $\text{HNO}_3 + \text{CH}_3\text{CO}$ | R1441 |
| | | $\text{CH}_3\text{CO} + \text{O}_2 \longrightarrow$ | R_Oxygen11/ |
| | | CH_3COO_2 | RRCOM |
| | | $\text{CH}_3\text{COO}_2 + \text{NO} \longrightarrow \text{CH}_3$ | D59/ |
| | | $+ \text{NO}_2 + \text{CO}_2$ | R4337 |

J.2 Bi-molecular reactions

Tropospheric chemistry module

| Reaction | Ref./CTM | |
|---|------------|--|
| O(¹D) | | |
| $\text{O}(^1\text{D}) + \text{O}_2 \longrightarrow \text{O}(^3\text{P}) + \text{O}_2$ | A3/R39M | |
| $\text{O}(^1\text{D}) + \text{H}_2\text{O} \longrightarrow 2\text{OH}$ | A6/R39H2OM | |
| $\text{O}(^1\text{D}) + \text{N}_2 \longrightarrow \text{O}(^3\text{P}) + \text{N}_2$ | A7/R39M | |
| HOx | | |
| $\text{O}_3 + \text{OH} \longrightarrow \text{O}_2 + \text{HO}_2$ | B6/R0140 | |
| $\text{OH} + \text{H}_2 \longrightarrow \text{H}_2\text{O} + \text{H}$ | B7/R1921 | |
| $\text{OH} + \text{HO}_2 \longrightarrow \text{H}_2\text{O} + \text{O}_2$ | B10/R4021 | |
| $\text{OH} + \text{H}_2\text{O}_2 \longrightarrow \text{H}_2\text{O} + \text{HO}_2$ | B11/R4015 | |
| $\text{O}_3 + \text{HO}_2 \longrightarrow \text{OH} + 2\text{O}_2$ | B12/R0121 | |
| $\text{HO}_2 + \text{HO}_2 \longrightarrow \text{H}_2\text{O}_2 + \text{O}_2$ | B13/R2121 | |
| $\text{HO}_2 + \text{HO}_2 + \text{M} \longrightarrow$ | | |
| $\text{H}_2\text{O}_2 + \text{O}_2 + \text{M}$ | B13/R2121 | |
| NOx | | |
| $\text{O}(^3\text{P}) + \text{NO}_2 \longrightarrow \text{NO} + \text{O}_2$ | C1/R3844 | |
| $\text{OH} + \text{HNO}_3 \longrightarrow \text{NO}_3 + \text{H}_2\text{O}$ | C9/R4004 | |
| $\text{NO} + \text{HO}_2 \longrightarrow \text{NO}_2 + \text{OH}$ | C12/R4321 | |
| $\text{OH} + \text{HO}_2\text{NO}_2 \longrightarrow$ | | |
| $\text{NO}_2 + \text{O}_2 + \text{HO}_2$ | C10/R4017 | |
| $\text{O}_3 + \text{NO} \longrightarrow \text{NO}_2 + \text{O}_2$ | C20/R0143 | |
| $\text{NO} + \text{NO}_3 \longrightarrow 2\text{NO}_2$ | C21/R4143 | |
| $\text{O}_3 + \text{NO}_2 \longrightarrow \text{NO}_3 + \text{O}_2$ | C22/R0144 | |
| $\text{NO}_2 + \text{NO}_3 \longrightarrow$ | | |
| $\text{NO} + \text{NO}_2 + \text{O}_2$ | C23/R4341B | |
| Organic | | |
| $\text{O}_3 + \text{C}_2\text{H}_4 \longrightarrow \text{HCHO}$ | D8/R0107 | |
| $+ 0.12\text{HO}_2 + 0.44\text{CO}$ | | |
| $\text{OH} + \text{CH}_4 \longrightarrow \text{CH}_3 + \text{H}_2\text{O}$ | D11/R4046 | |
| $\text{OH} + \text{C}_2\text{H}_6 \longrightarrow$ | D21/R4008 | |
| $\text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$ | | |
| $\text{O}_3 + \text{C}_3\text{H}_6 \longrightarrow 0.25\text{HO}_2$ | Ox_VOC6/ | |
| $+ 0.5(\text{HCHO} + \text{CH}_3\text{CHO})$ | R0109 | |
| $+ 0.15\text{OH} + 0.03\text{CH}_3\text{O}$ | | |
| $+ 0.31\text{CH}_3 + 0.07\text{CH}_4$ | | |
| $+ 0.4\text{CO}$ | | |

| <div>CH₃COO₂ + CH₃O₂ → CH₃O + CH₃ + CO₂ + O₂ CH₃COO₂ + CH₃O₂ → HCHO + CH₃COOH + O₂ CH₃O₂ + C₂H₅O₂ → 0.5(CH₃O + (1-fb₆₈)(HCHO + CH₃) + fb₆₈ (HO₂ + CH₃CHO)) + 0.25(HCHO + CH₃CHO) CH₃O₂ + C₃H₇O₂ → 0.5(CH₃O + (1-fb₆₉)(CH₃CHO + CH₃O₂) + fb₆₉(HO₂ + CH₃COCH₃)) + 0.25(HCHO + CH₃COCH₃) CH₃O₂ + C₄H₉O₂ → 0.5(CH₃O + (1-fb₇₀)(CH₃CHO + C₂H₅O₂) + fb₇₀(HO₂ + CH₃COCH₂CH₃)) + 0.25(HCHO + CH₃COCH₂CH₃) CH₃O₂ + C₆H₁₃O₂ → CH₃O + CH₃CHO + C₄H₉O₂ CH₃O₂ + CH₃COCH₂(O₂) → CH₃O + CH₃COCHO + HCHO + HO₂ CH₃O₂ + CH₃CH(O₂)CH₂OH → CH₃O + CH₃CHO + HCHO + HO₂ CH₃O₂ + CH₃COCH(O₂)CH₃ → CH₃O + HO₂ + CH₃COCOCH₃ CH₃O₂ + ISOR1 → HCHO + CH₃O + HO₂ + ISOK CH₃O₂ + ISOR2 → RCOHCO + CH₃O + HO₂ HO₂ + CH₃O(O₂) → CH₃O₂H + O₂ HO₂ + C₂H₅O₂ → CH₃O₂H HO₂ + C₃H₇O₂ → CH₃O₂H HO₂ + C₄H₉O₂ → CH₃O₂H HO₂ + C₆H₁₃O₂ → CH₃O₂H HO₂ + CH₃COCH₂(O₂) → CH₃O₂H HO₂ + CH₃CH(O₂)CH₂OH → CH₃O₂H HO₂ + CH₃COCH(O₂)CH₃ → CH₃O₂H HO₂ + ISOR1 → CH₃O₂H HO₂ + ISOR2 → CH₃O₂H</div> | <div>D52/<i>ROO_23</i>/ R2237A D52/<i>ROO_23</i>/ R2237A ROO_41/ R2223 use ROO_41/ R2249 use ROO_41/ R2224 use ROO_41/ R2225 ROO_24/ R2251 use ROO_41/ R2228 R2227 use ROO_41/ R22AR use ROO_41/ R22AR HOx_VOC54/ R2137 D36/RARAD D36/RARAD D36/RARAD D36/RARAD D36/<i>HOx_VOC57</i>/ RARAD use D36/ RARAD use D36/ RARAD use D36/RARAD use D36/RARAD</div> | <div>Stratospheric chemistry module</div> <table><thead><tr><th>Reaction</th><th>Ref./CTM</th></tr></thead><tbody><tr><td>Ox</td><td></td></tr><tr><td>O(³P) + O₃ → O₂ + O₂</td><td>A1/C107</td></tr><tr><td>O(¹D)</td><td></td></tr><tr><td>O(¹D) + N₂O → N₂ + O₂</td><td>A8/C213A</td></tr><tr><td>O(¹D) + N₂O → NO + NO</td><td>A7/C213B</td></tr><tr><td>O(¹D) + H₂O → OH + OH</td><td>A6/C222</td></tr><tr><td>O(¹D) + CH₄ → OH + CH₃</td><td>A11/C256A,B</td></tr><tr><td>O(¹D) + CH₄ → HCHO + H₂</td><td>A11/C256C</td></tr><tr><td>O(¹D) + H₂ → OH + H</td><td>A5/C221</td></tr><tr><td>O(¹D) + N₂ → O(³P) + N₂</td><td>A7/R2M</td></tr><tr><td>O(¹D) + O₂ → O(³P) + O₂</td><td>A3/R2M</td></tr><tr><td>O(¹D) + HCl → Cl + OH</td><td>A12/C239</td></tr><tr><td>O(¹D) + CFC1₃ → Clx</td><td>A19/C261A</td></tr><tr><td>O(¹D) + CF₂Cl₂ → Clx</td><td>A20/C261B</td></tr><tr><td>O(¹D) + CHCl₂CF₃ → Clx</td><td>A42/CHCFC123OD</td></tr><tr><td>O(¹D) + CH₃CCl₂F → Clx</td><td>A36/CHCFC141OD</td></tr><tr><td>O(¹D) + CH₃CClF₂ → Clx</td><td>A37/CHCFC142OD</td></tr><tr><td>HOx</td><td></td></tr><tr><td>O(³P) + OH → O₂ + H</td><td>B1/R119</td></tr><tr><td>O(³P) + HO₂ → OH + O₂</td><td>B2/R120</td></tr><tr><td>H + O₃ → OH + O₂</td><td>B4/C718</td></tr><tr><td>H + HO₂ → 2OH</td><td>B5/CHHO2A</td></tr><tr><td>H + HO₂ → O + H₂O</td><td>B5/CHHO2B</td></tr><tr><td>H + HO₂ → H₂ + O₂</td><td>B5/CHHO2C</td></tr><tr><td>OH + O₃ → HO₂ + O₂</td><td>B6/C719</td></tr><tr><td>OH + H₂ → H₂O + H</td><td>B7/C1921</td></tr><tr><td>OH + OH → H₂O + O(³P)</td><td>B9/C1919</td></tr><tr><td>OH + HO₂ → H₂O + O₂</td><td>B10/C1920</td></tr><tr><td>OH + H₂O₂ → H₂O + HO₂</td><td>B11/C1923</td></tr><tr><td>HO₂ + O₃ → OH + 2O₂</td><td>B12/C720</td></tr><tr><td>HO₂ + HO₂ → H₂O₂ + O₂</td><td>B13/R2020</td></tr><tr><td>HO₂ + HO₂ + M → H₂O₂ + O₂ + M</td><td>B13/R2020</td></tr><tr><td>NOx</td><td></td></tr><tr><td>O(³P) + NO₂ → NO + O₂</td><td>C1/C110</td></tr><tr><td>OH + HNO₃ → H₂O + NO₃</td><td>C9/C1926</td></tr><tr><td>OH + HO₂NO₂ → O₂ + H₂O + NO₂</td><td>C10/C191020</td></tr><tr><td>NO + HO₂ → NO₂ + OH</td><td>C12/C920</td></tr><tr><td>N + O₂ → NO + O(³P)</td><td>C16/RC2</td></tr><tr><td>N + NO → N₂ + O(³P)</td><td>C18/RC1</td></tr><tr><td>O₃ + NO → NO₂ + O₂</td><td>C20/C709</td></tr><tr><td>NO + NO₃ → 2NO₂</td><td>C21/C911</td></tr><tr><td>O₃ + NO₂ → NO₃ + O₂</td><td>C22/C710</td></tr><tr><td>NO₂ + NO₃ → NO + NO₂ + O₂</td><td>C23/C1011</td></tr><tr><td>Organic</td><td></td></tr><tr><td>O(³P) + HCHO → HCO + OH</td><td>D4/R148</td></tr><tr><td>OH + CH₄ → CH₃ + H₂O</td><td>D11/C1956</td></tr><tr><td>OH + HCHO → H₂O + HCO</td><td>D14/C1948</td></tr><tr><td>OH + CH₃O₂H → 0.7 (CH₃O₂ + H₂O)</td><td>D16/C19CX</td></tr><tr><td>OH + CH₃O₂H → 0.3 (CH₂O + OH + H₂O)</td><td>D16/C19CX</td></tr><tr><td>HO₂ + CH₃O₂ → CH₃OOH + O₂</td><td>D35/R2051</td></tr><tr><td>CH₃O₂ + NO → CH₃O + NO₂</td><td>D51/C951C</td></tr><tr><td>ClOx</td><td></td></tr><tr><td>O(³P) + ClO → Cl + O₂</td><td>F1/C136</td></tr><tr><td>O(³P) + OClO → ClO + O₂</td><td>F2/C60B</td></tr><tr><td>O(³P) + HCl → OH + Cl</td><td>F4/C139</td></tr><tr><td>O(³P) + ClONO₂ → NO₃ + ClO</td><td>F6/C143A</td></tr><tr><td>OH + ClO → HO₂ + Cl</td><td>F10/C1936A</td></tr><tr><td>OH + ClO → HCl + O₂</td><td>F10/C1936B</td></tr><tr><td>OH + HCl → H₂O + Cl</td><td>F12/C1939</td></tr><tr><td>OH + OHCl → H₂O + ClO</td><td>F13/C1937</td></tr><tr><td>OH + ClONO₂ → OHCl + NO₃</td><td>F15/C1943A</td></tr><tr><td>OH + CH₃Cl → Clx</td><td>F16/C1961C</td></tr><tr><td>OH + CHF₂Cl → Clx</td><td>F22/C1965B</td></tr><tr><td>OH + CH₃CCl₃ → Clx</td><td>F26/1965A</td></tr><tr><td>OH + CH₃CCl₂F → Clx</td><td>F27/RHCFC141OH</td></tr><tr><td>OH + CH₃CClF₂ → Clx</td><td>F28/RHCFC142OH</td></tr><tr><td>OH + CHCl₂CF₃ → Clx</td><td>F33/RHCFC123OH</td></tr><tr><td>HO₂ + Cl → HCl + O₂</td><td>F45/R2035</td></tr><tr><td>HO₂ + Cl → OH + ClO</td><td>F45/R2035B</td></tr><tr><td>HO₂ + ClO → OHCl + O₂</td><td>F46/R2036</td></tr></tbody></table> | Reaction | Ref./CTM | Ox | | O(³ P) + O ₃ → O ₂ + O ₂ | A1/C107 | O(¹D) | | O(¹ D) + N ₂ O → N ₂ + O ₂ | A8/C213A | O(¹ D) + N ₂ O → NO + NO | A7/C213B | O(¹ D) + H ₂ O → OH + OH | A6/C222 | O(¹ D) + CH ₄ → OH + CH ₃ | A11/C256A,B | O(¹ D) + CH ₄ → HCHO + H ₂ | A11/C256C | O(¹ D) + H ₂ → OH + H | A5/C221 | O(¹ D) + N ₂ → O(³ P) + N ₂ | A7/R2M | O(¹ D) + O ₂ → O(³ P) + O ₂ | A3/R2M | O(¹ D) + HCl → Cl + OH | A12/C239 | O(¹ D) + CFC1 ₃ → Clx | A19/C261A | O(¹ D) + CF ₂ Cl ₂ → Clx | A20/C261B | O(¹ D) + CHCl ₂ CF ₃ → Clx | A42/CHCFC123OD | O(¹ D) + CH ₃ CCl ₂ F → Clx | A36/CHCFC141OD | O(¹ D) + CH ₃ CClF ₂ → Clx | A37/CHCFC142OD | HOx | | O(³ P) + OH → O ₂ + H | B1/R119 | O(³ P) + HO ₂ → OH + O ₂ | B2/R120 | H + O ₃ → OH + O ₂ | B4/C718 | H + HO ₂ → 2OH | B5/CHHO2A | H + HO ₂ → O + H ₂ O | B5/CHHO2B | H + HO ₂ → H ₂ + O ₂ | B5/CHHO2C | OH + O ₃ → HO ₂ + O ₂ | B6/C719 | OH + H ₂ → H ₂ O + H | B7/C1921 | OH + OH → H ₂ O + O(³ P) | B9/C1919 | OH + HO ₂ → H ₂ O + O ₂ | B10/C1920 | OH + H ₂ O ₂ → H ₂ O + HO ₂ | B11/C1923 | HO ₂ + O ₃ → OH + 2O ₂ | B12/C720 | HO ₂ + HO ₂ → H ₂ O ₂ + O ₂ | B13/R2020 | HO ₂ + HO ₂ + M → H ₂ O ₂ + O ₂ + M | B13/R2020 | NOx | | O(³ P) + NO ₂ → NO + O ₂ | C1/C110 | OH + HNO ₃ → H ₂ O + NO ₃ | C9/C1926 | OH + HO ₂ NO ₂ → O ₂ + H ₂ O + NO ₂ | C10/C191020 | NO + HO ₂ → NO ₂ + OH | C12/C920 | N + O ₂ → NO + O(³ P) | C16/RC2 | N + NO → N ₂ + O(³ P) | C18/RC1 | O ₃ + NO → NO ₂ + O ₂ | C20/C709 | NO + NO ₃ → 2NO ₂ | C21/C911 | O ₃ + NO ₂ → NO ₃ + O ₂ | C22/C710 | NO ₂ + NO ₃ → NO + NO ₂ + O ₂ | C23/C1011 | Organic | | O(³ P) + HCHO → HCO + OH | D4/R148 | OH + CH ₄ → CH ₃ + H ₂ O | D11/C1956 | OH + HCHO → H ₂ O + HCO | D14/C1948 | OH + CH ₃ O ₂ H → 0.7 (CH ₃ O ₂ + H ₂ O) | D16/C19CX | OH + CH ₃ O ₂ H → 0.3 (CH ₂ O + OH + H ₂ O) | D16/C19CX | HO ₂ + CH ₃ O ₂ → CH ₃ OOH + O ₂ | D35/R2051 | CH ₃ O ₂ + NO → CH ₃ O + NO ₂ | D51/C951C | ClOx | | O(³ P) + ClO → Cl + O ₂ | F1/C136 | O(³ P) + OClO → ClO + O ₂ | F2/C60B | O(³ P) + HCl → OH + Cl | F4/C139 | O(³ P) + ClONO ₂ → NO ₃ + ClO | F6/C143A | OH + ClO → HO ₂ + Cl | F10/C1936A | OH + ClO → HCl + O ₂ | F10/C1936B | OH + HCl → H ₂ O + Cl | F12/C1939 | OH + OHCl → H ₂ O + ClO | F13/C1937 | OH + ClONO ₂ → OHCl + NO ₃ | F15/C1943A | OH + CH ₃ Cl → Clx | F16/C1961C | OH + CHF ₂ Cl → Clx | F22/C1965B | OH + CH ₃ CCl ₃ → Clx | F26/1965A | OH + CH ₃ CCl ₂ F → Clx | F27/RHCFC141OH | OH + CH ₃ CClF ₂ → Clx | F28/RHCFC142OH | OH + CHCl ₂ CF ₃ → Clx | F33/RHCFC123OH | HO ₂ + Cl → HCl + O ₂ | F45/R2035 | HO ₂ + Cl → OH + ClO | F45/R2035B | HO ₂ + ClO → OHCl + O ₂ | F46/R2036 |
|--|--|---|----------|----------|-----------|--|---|---------|-------------------------|--|---|----------|---|----------|---|---------|---|-------------|--|-----------|--|---------|---|--------|---|--------|------------------------------------|----------|--|-----------|--|-----------|--|----------------|---|----------------|--|----------------|------------|--|--|---------|--|---------|--|---------|---------------------------|-----------|--|-----------|---|-----------|--|---------|--|----------|---|----------|--|-----------|---|-----------|---|----------|--|-----------|---|-----------|------------|--|--|---------|--|----------|---|-------------|---|----------|--|---------|--|---------|--|----------|---|----------|---|----------|--|-----------|----------------|--|--------------------------------------|---------|---|-----------|------------------------------------|-----------|--|-----------|--|-----------|---|-----------|---|-----------|-------------|--|--|---------|--|---------|------------------------------------|---------|---|----------|---------------------------------|------------|---------------------------------|------------|----------------------------------|-----------|------------------------------------|-----------|--|------------|-------------------------------|------------|--------------------------------|------------|---|-----------|---|----------------|--|----------------|--|----------------|---|-----------|---------------------------------|------------|---|-----------|
| Reaction | Ref./CTM | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| Ox | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| O(³ P) + O ₃ → O ₂ + O ₂ | A1/C107 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| O(¹D) | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| O(¹ D) + N ₂ O → N ₂ + O ₂ | A8/C213A | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| O(¹ D) + N ₂ O → NO + NO | A7/C213B | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| O(¹ D) + H ₂ O → OH + OH | A6/C222 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| O(¹ D) + CH ₄ → OH + CH ₃ | A11/C256A,B | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| O(¹ D) + CH ₄ → HCHO + H ₂ | A11/C256C | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| O(¹ D) + H ₂ → OH + H | A5/C221 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| O(¹ D) + N ₂ → O(³ P) + N ₂ | A7/R2M | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| O(¹ D) + O ₂ → O(³ P) + O ₂ | A3/R2M | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| O(¹ D) + HCl → Cl + OH | A12/C239 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| O(¹ D) + CFC1 ₃ → Clx | A19/C261A | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| O(¹ D) + CF ₂ Cl ₂ → Clx | A20/C261B | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| O(¹ D) + CHCl ₂ CF ₃ → Clx | A42/CHCFC123OD | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| O(¹ D) + CH ₃ CCl ₂ F → Clx | A36/CHCFC141OD | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| O(¹ D) + CH ₃ CClF ₂ → Clx | A37/CHCFC142OD | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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| O(³ P) + OH → O ₂ + H | B1/R119 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| O(³ P) + HO ₂ → OH + O ₂ | B2/R120 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| H + O ₃ → OH + O ₂ | B4/C718 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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| OH + OH → H ₂ O + O(³ P) | B9/C1919 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| OH + HO ₂ → H ₂ O + O ₂ | B10/C1920 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| OH + H ₂ O ₂ → H ₂ O + HO ₂ | B11/C1923 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| HO ₂ + O ₃ → OH + 2O ₂ | B12/C720 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| HO ₂ + HO ₂ → H ₂ O ₂ + O ₂ | B13/R2020 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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| O(³ P) + NO ₂ → NO + O ₂ | C1/C110 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| OH + HNO ₃ → H ₂ O + NO ₃ | C9/C1926 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| OH + HO ₂ NO ₂ → O ₂ + H ₂ O + NO ₂ | C10/C191020 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| NO + HO ₂ → NO ₂ + OH | C12/C920 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| N + O ₂ → NO + O(³ P) | C16/RC2 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| N + NO → N ₂ + O(³ P) | C18/RC1 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| O ₃ + NO → NO ₂ + O ₂ | C20/C709 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| NO + NO ₃ → 2NO ₂ | C21/C911 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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| O(³ P) + HCHO → HCO + OH | D4/R148 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| OH + CH ₄ → CH ₃ + H ₂ O | D11/C1956 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| OH + HCHO → H ₂ O + HCO | D14/C1948 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| OH + CH ₃ O ₂ H → 0.7 (CH ₃ O ₂ + H ₂ O) | D16/C19CX | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| OH + CH ₃ O ₂ H → 0.3 (CH ₂ O + OH + H ₂ O) | D16/C19CX | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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| CH ₃ O ₂ + NO → CH ₃ O + NO ₂ | D51/C951C | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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| O(³ P) + ClO → Cl + O ₂ | F1/C136 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| O(³ P) + OClO → ClO + O ₂ | F2/C60B | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| O(³ P) + HCl → OH + Cl | F4/C139 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| O(³ P) + ClONO ₂ → NO ₃ + ClO | F6/C143A | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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| OH + HCl → H ₂ O + Cl | F12/C1939 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| OH + OHCl → H ₂ O + ClO | F13/C1937 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| OH + ClONO ₂ → OHCl + NO ₃ | F15/C1943A | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| OH + CH ₃ Cl → Clx | F16/C1961C | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| OH + CHF ₂ Cl → Clx | F22/C1965B | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| OH + CH ₃ CCl ₃ → Clx | F26/1965A | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| OH + CH ₃ CCl ₂ F → Clx | F27/RHCFC141OH | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| OH + CH ₃ CClF ₂ → Clx | F28/RHCFC142OH | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| OH + CHCl ₂ CF ₃ → Clx | F33/RHCFC123OH | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| HO ₂ + Cl → HCl + O ₂ | F45/R2035 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| HO ₂ + Cl → OH + ClO | F45/R2035B | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| HO ₂ + ClO → OHCl + O ₂ | F46/R2036 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

| | |
|---|------------|
| $\text{NO} + \text{OCIO} \longrightarrow \text{NO}_2 + \text{ClO}$ | F48/C60A |
| $\text{Cl} + \text{O}_3 \longrightarrow \text{ClO} + \text{O}_2$ | F52/C735 |
| $\text{Cl} + \text{H}_2 \longrightarrow \text{HCl} + \text{H}$ | F53/C2135 |
| $\text{Cl} + \text{H}_2\text{O}_2 \longrightarrow \text{HCl} + \text{HO}_2$ | F54/C2335 |
| $\text{Cl} + \text{CH}_4 \longrightarrow \text{HCl} + \text{CH}_3$ | F59/C3556 |
| $\text{Cl} + \text{HCHO} \longrightarrow \text{HCl} + \text{HCO}$ | F61/C3548 |
| $\text{Cl} + \text{ClONO}_2 \longrightarrow 2\text{Cl} + \text{NO}_3$ | F85/C3543A |
| $\text{ClO} + \text{NO} \longrightarrow \text{NO}_2 + \text{Cl}$ | F111/C936 |
| $\text{ClO} + \text{CO} \longrightarrow \text{Cl} + \text{CO}_2$ | F114/C3645 |
| BrOx | |
| $\text{O}(^3\text{P}) + \text{BrO} \longrightarrow \text{Br} + \text{O}_2$ | G1/C51A |
| $\text{O}(^3\text{P}) + \text{HBr} \longrightarrow \text{OH} + \text{Br}$ | G2/C52B |
| $\text{OH} + \text{Br}_2 \longrightarrow \text{OHBr} + \text{Br}$ | G5/C53A |
| $\text{OH} + \text{BrO} \longrightarrow \text{HBr} + \text{O}_2$ | G6/C51J |
| $\text{OH} + \text{BrO} \longrightarrow \text{Br} + \text{HO}_2$ | G6/C51K |
| $\text{OH} + \text{HBr} \longrightarrow \text{H}_2\text{O} + \text{Br}$ | G7/C52A |
| $\text{OH} + \text{CH}_3\text{Br} \longrightarrow \text{Bry}$ | G8/C19MBr |
| $\text{HO}_2 + \text{Br} \longrightarrow \text{HBr} + \text{O}_2$ | G24/C50D |
| $\text{HO}_2 + \text{BrO} \longrightarrow \text{OHBr} + \text{O}_2$ | G25/C51I |
| $\text{Br} + \text{O}_3 \longrightarrow \text{BrO} + \text{O}_2$ | G31/C50A |
| $\text{Br} + \text{H}_2\text{O}_2 \longrightarrow \text{HBr} + \text{HO}_2$ | G32/C50B |
| $\text{Br} + \text{HCHO} \longrightarrow \text{HBr} + \text{CHO}$ | G34/C50C |
| $\text{BrO} + \text{O}_3 \longrightarrow \text{Br} + 2\text{O}_2$ | G38/C51H |
| $\text{BrO} + \text{NO} \longrightarrow \text{NO}_2 + \text{Br}$ | G39/C51D |
| $\text{BrO} + \text{ClO} \longrightarrow \text{Br} + \text{OCIO}$ | G41/C51B |
| $\text{BrO} + \text{ClO} \longrightarrow \text{Br} + \text{ClOO}$ | G41/C51C |
| $\text{BrO} + \text{ClO} \longrightarrow \text{BrCl} + \text{O}_2$ | G41/C51L |
| $\text{BrO} + \text{BrO} \longrightarrow 2\text{Br} + \text{O}_2$ | G42/C51F |
| $\text{BrO} + \text{BrO} \longrightarrow \text{Br}_2 + \text{O}_2$ | G42/C51G |

J.3 Tri-molecular reactions

Tropospheric chemistry module

| Reaction | Ref./CTM |
|---|------------------------|
| Ox | |
| $\text{O}(^3\text{P}) + \text{O}_2 + \text{M} \longrightarrow \text{O}_3 + \text{M}$ | |
| HOx | |
| $\text{OH} + \text{OH} + \text{M} \longrightarrow \text{H}_2\text{O}_2$ | B2/R4040M |
| $\text{HO}_2 + \text{HO}_2 + \text{M} \longrightarrow \text{H}_2\text{O}_2 + \text{O}_2 + \text{M}$ | See bi-molecular |
| NOx | |
| $\text{OH} + \text{NO}_2 + \text{M} \longrightarrow \text{HNO}_3 + \text{M}$ | C4/R4440 |
| $\text{NO}_2 + \text{HO}_2 + \text{M} \longrightarrow \text{HO}_2\text{NO}_2 + \text{M}$ | C5/R4421 |
| $\text{NO}_2 + \text{NO}_3 + \text{M} \longrightarrow \text{N}_2\text{O}_5 + \text{M}$ | C6/R4441A |
| $\text{HO}_2\text{NO}_2 + \text{M} \longrightarrow \text{HO}_2 + \text{NO}_2 + \text{M}$ | NOx17/R17T |
| $\text{N}_2\text{O}_5 + \text{M} \longrightarrow \text{NO}_2 + \text{NO}_3 + \text{M}$ | NOx32/R42T |
| Organic | |
| $\text{OH} + \text{CO} + \text{O}_2 \longrightarrow \text{HO}_2 + \text{CO}_2$ | HOx_VOC10/ R4006 |
| $\text{OH} + \text{C}_2\text{H}_4 + \text{M} \longrightarrow \text{CH}_3 + \text{HCHO} + \text{M}$ | D5/ R4007 |
| $\text{OH} + \text{C}_3\text{H}_6 + \text{M} \longrightarrow \text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + \text{M}$ | /HOx_VOC5/ R4009 |
| $\text{CH}_3 + \text{O}_2 + \text{M} \longrightarrow \text{CH}_3\text{O}_2 + \text{M}$ | D3/R_Oxygen1/ RCH3M |
| $\text{CH}_3\text{COO}_2 + \text{NO}_2 + \text{M} \longrightarrow \text{PAN} + \text{M}$ | D12/ R4437 |
| $\text{PAN} + \text{M} \longrightarrow \text{CH}_3\text{COO}_2 + \text{NO}_2 + \text{M}$ | ROO_15/ R5T |

Stratospheric chemistry module

| Reaction | Ref./CTM |
|---|---------------------|
| Ox | |
| $\text{O}(^3\text{P}) + \text{O}_2 + \text{M} \longrightarrow \text{O}_3 + \text{M}$ | A1/C104M |
| HOx | |
| $\text{H} + \text{O}_2 + \text{M} \longrightarrow \text{HO}_2 + \text{M}$ | B1/C418M |
| $\text{OH} + \text{OH} + \text{M} \longrightarrow \text{H}_2\text{O} + \text{O}(^3\text{P}) + \text{M}$ | B2/C1919M |
| NOx | |
| $\text{O}(^3\text{P}) + \text{NO}_2 + \text{M} \longrightarrow \text{NO}_3 + \text{M}$ | C2/C110M |
| $\text{OH} + \text{NO}_2 + \text{M} \longrightarrow \text{HNO}_3 + \text{M}$ | C4/C1019X |
| $\text{NO}_2 + \text{HO}_2 + \text{M} \longrightarrow \text{HO}_2\text{NO}_2 + \text{M}$ | C5/C1020 |
| $\text{NO}_2 + \text{NO}_3 + \text{M} \longrightarrow \text{N}_2\text{O}_5 + \text{M}$ | C6/C1011X |
| Organic | |
| $\text{OH} + \text{CO} + \text{O}_2 \longrightarrow \text{HO} + \text{CO}_2$ | HOx_VOC10/ C1945 |
| ClOx | |
| $\text{Cl} + \text{O}_2 + \text{M} \longrightarrow \text{ClOO} + \text{M}$ | F1/C3504 |
| $\text{ClO} + \text{NO}_2 + \text{M} \longrightarrow \text{ClONO}_2 + \text{M}$ | F8/C1036M |
| $\text{ClO} + \text{ClO} + \text{M} \longrightarrow \text{Cl}_2\text{O}_2 + \text{M}$ | F10/C36M |
| BrOx | |
| $\text{BrO} + \text{NO}_2 + \text{M} \longrightarrow \text{BrONO}_2 + \text{M}$ | G2/C51E |

J.4 Instantaneous reactions

Stratospheric chemistry module

| Reaction | Ref./CTM |
|--|----------------|
| $\text{CH}_3 + \text{O}_2 \longrightarrow \text{CH}_3\text{O}_2$ | D42/R_Oxygen1 |
| $\text{HCO} + \text{O}_2 \longrightarrow \text{CO} + \text{HO}_2$ | D44/R_Oxygen10 |
| $\text{CH}_3\text{O} + \text{O}_2 \longrightarrow \text{CH}_2\text{O} + \text{HO}_2$ | D46/R_O1 |

J.5 Thermal decomposition reactions

Stratospheric chemistry module

| Reaction | JPL Ref./CTM |
|--|---------------|
| $\text{HO}_2\text{NO}_2 \longrightarrow \text{HO}_2 + \text{NO}_2$ | T3-1.2/CC1020 |
| $\text{N}_2\text{O}_5 \longrightarrow \text{NO}_2 + \text{NO}_3$ | T3-1.4/C14M |
| $\text{ClOO} \longrightarrow \text{Cl} + \text{O}_2$ | T3-1.11/C61A |
| $\text{Cl}_2\text{O}_2 \longrightarrow \text{ClO} + \text{ClO}$ | T3-1.14/C61B |

J.6 Heterogeneous reactions

Tropospheric chemistry module

| Reaction | Ref./CTM |
|--|------------|
| $\text{N}_2\text{O}_5 + \text{aq(aerosol)} \longrightarrow 2\text{HNO}_3(\text{aq})$ | NA/PR42HET |

Stratospheric chemistry moduleSee the code in *oc_stratchem_rates.f* for full references.

| Reaction | CTM |
|---|----------|
| On PSCs | |
| $\text{N}_2\text{O}_5 + \text{HCl} (\text{s}) \longrightarrow \text{ClONO}_2 + \text{HNO}_3 (\text{s})$ | ACPAR |
| $\text{N}_2\text{O}_5 + \text{H}_2\text{O} (\text{s}) \longrightarrow 2\text{HNO}_3 (\text{s})$ | ADPAR |
| $\text{ClONO}_2 + \text{HCl} (\text{s}) \longrightarrow \text{Cl}_2 + \text{HNO}_3 (\text{s})$ | BCPAR |
| $\text{ClONO}_2 + \text{H}_2\text{O} (\text{s}) \longrightarrow \text{HOCl} + \text{HNO}_3 (\text{s})$ | BDPAR |
| $\text{HOCl} + \text{HCl} (\text{s}) \longrightarrow \text{Cl}_2 + \text{H}_2\text{O} (\text{s})$ | ECPAR |
| $\text{BrONO}_2 + \text{H}_2\text{O} (\text{s}) \longrightarrow \text{OHBr} + \text{HNO}_3 (\text{s})$ | FDPAR |
| $\text{BrONO}_2 + \text{HCl} (\text{s}) \longrightarrow \text{BrCl} + \text{HNO}_3 (\text{s})$ | FCPAR |
| $\text{OHBr} + \text{HCl} (\text{s}) \longrightarrow \text{BrCl} + \text{H}_2\text{O} (\text{s})$ | GCPAR |
| $\text{ClONO}_2 + \text{HBr} (\text{s}) \longrightarrow \text{BrCl} + \text{H}_2\text{O} (\text{s})$ | BHPAR |
| On sulfuric aerosols | |
| $\text{N}_2\text{O}_5 + \text{HCl} \longrightarrow \text{ClONO}_2 + \text{HNO}_3$ | /ACPARBK |
| $\text{N}_2\text{O}_5 + \text{H}_2\text{O} \longrightarrow 2\text{HNO}_3$ | ADPARBK |
| $\text{ClONO}_2 + \text{HCl} \longrightarrow \text{Cl}_2 + \text{HNO}_3$ | BCPARBK |
| $\text{ClONO}_2 + \text{H}_2\text{O} \longrightarrow \text{HOCl} + \text{HNO}_3$ | BDPARBK |
| $\text{HOCl} + \text{HCl} \longrightarrow \text{Cl}_2 + \text{H}_2\text{O}$ | ECPARBK |
| $\text{BrONO}_2 + \text{H}_2\text{O} \longrightarrow \text{OHBr} + \text{HNO}_3$ | FDPARBK |
| $\text{BrONO}_2 + \text{HCl} \longrightarrow \text{BrCl} + \text{HNO}_3$ | FCPARBK |
| $\text{OHBr} + \text{HCl} \longrightarrow \text{BrCl} + \text{H}_2\text{O}$ | GCPARBK |

For reactions on PSCs, the species marked (s) stay on the particle.

Relationships between process sensitivity in HadGEM3-UKCA and inter-model variation from AeroCom Phase II (Kipling et al., 2016).

Evaluation of the aerosol vertical distribution in global aerosol models through comparison against CALIOP measurements: AeroCom phase II results (Koffi et al., 2016).

Evaluation of observed and modelled aerosol lifetimes using radioactive tracers of opportunity and an ensemble of 19 global models (Kristiansen et al., 2016).

Extensive release of methane from Arctic seabed west of Svalbard during summer 2014 does not influence the atmosphere (Myhre et al., 2016).

Comparison of aerosol optical properties above clouds between POLDER and AeroCom models over the South East Atlantic Ocean during the fire season (Peers et al., 2016).

Radiative forcing from aircraft emissions of NO_x: model calculations with CH₄ surface flux boundary condition (Pitari et al., 2016).

Multi-model evaluation of short-lived pollutant distributions over East Asia during summer 2008 (Quennehen et al., 2016).

The effect of future ambient air pollution on human premature mortality to 2100 using output from the ACCMIP model ensemble (Silva et al., 2016).

Global and regional radiative forcing from 20% reductions in BC, OC and SO₄ - an HTAP2 multi-model study (Stjern et al., 2016).

K Peer-reviewed papers

Here you find the peer-reviewed papers of Oslo CTM3 and Oslo CTM2. and a few older Oslo CTM1 papers at the end.

K.1 2017 – 6 papers

Regional temperature change potentials for short-lived climate forcers based on radiative forcing from multiple models (Aamaas et al., 2017).

Investigation of global particulate nitrate from the AeroCom phase III experiment (Bian et al., 2017).

Emission metrics for quantifying regional climate impacts of aviation (Lund et al., 2017a).

Sensitivity of black carbon concentrations and climate impact to aging and scavenging in OsloCTM2-M7 (Lund et al., 2017b).

Multi-model simulations of aerosol and ozone radiative forcing due to anthropogenic emission changes during the period 1990-2015 (Myhre et al., 2017).

Aerosols at the poles: an AeroCom Phase II multi-model evaluation (Sand et al., doi:10.5194/acp-17-12197-2017).

K.2 2016 – 11 papers

Regional emission metrics for short-lived climate forcers from multiple models (Aamaas et al., 2016).

Atmospheric methane evolution the last 40 years (Dalsøren et al., 2016).

What controls the vertical distribution of aerosol?

K.3 2015 – 5 papers

AMAP Assessment 2015: Methane as an Arctic climate forcer (Arctic Monitoring and Assessment Programme (AMAP), 2015).

Current model capabilities for simulating black carbon and sulfate concentrations in the Arctic atmosphere: a multi-model evaluation using a comprehensive measurement data set (Eckhardt et al., 2015).

Impact of coupled NO_x-aerosol aircraft emissions on ozone photochemistry and radiative forcing (Pitari et al., 2015).

Measuring and Modeling the Lifetime of Nitrous Oxide including its Variability (Prather et al., 2015).

Evaluating the climate and air quality impacts of short-lived pollutants (Stohl et al., 2015).

K.4 2014 – 11 papers

Forty-seven years of weekly atmospheric black carbon measurements in the Finnish Arctic: Decrease in black carbon with declining emissions (Dutkiewicz et al., 2014).

Climate penalty for shifting shipping to the Arctic (Fuglestad et al., 2014).

How shorter black carbon lifetime alters its climate effect (Hodnebrog et al., 2014).

Atmospheric Ozone and Methane in a Changing Climate (Isaksen et al., 2014).

An AeroCom assessment of black carbon in Arctic snow and sea ice (Jiao et al., 2014).

Climate impacts of short-lived climate forcers versus CO₂ from biodiesel: A case of the EU on-road sector (Lund et al., 2014a).

Global and regional climate impacts of black carbon and co-emitted species from the on-road diesel sector (Lund et al., 2014b).

Modelled black carbon radiative forcing and atmospheric lifetime in AeroCom Phase II constrained by aircraft observations (Samset et al., 2014).

Aircraft emission mitigation by changing route altitude: A multi-model estimate of aircraft NO_x emission impact on O₃ photochemistry (Søvde et al., 2014).

The AeroCom evaluation and intercomparison of organic aerosol in global models (Tsigaridis et al., 2014).

The influence of future non-mitigated road transport emissions on regional ozone exceedences at global scale (Williams et al., 2014).

K.5 2013 – 20 papers

Evaluation of ACCMIP outgoing longwave radiation from tropospheric ozone using TES satellite observations (Bowman et al., 2013).

Environmental impacts of shipping in 2030 with a particular focus on the Arctic region (Dalsøren et al., 2013).

Reducing CO₂ from shipping - do non-CO₂ effects matter? (Eide et al., 2013).

Ozone Variations Derived by a Chemical Transport Model (Eleftheratos et al., 2013).

Elemental carbon measurements in European Arctic snow packs (Forsström et al., 2013).

Improvements to the retrieval of tropospheric NO₂

from satellite stratospheric correction using SCIAMACHY limb/nadir matching and comparison to Oslo CTM2 simulations (Hilboll et al., 2013).

Global Warming Potentials and Radiative Efficiencies of Halocarbons and Related Compounds: A Comprehensive Review (Hodnebrog et al., 2013).

Future methane, hydroxyl, and their uncertainties: key climate and emission parameters for future predictions (Holmes et al., 2013).

Multi-model mean nitrogen and sulfur deposition from the Atmospheric Chemistry and Climate Model Intercomparison Project (ACCMIP): evaluation of historical and projected future changes (Lamarque et al., 2013a).

The Atmospheric Chemistry and Climate Model Intercomparison Project (ACCMIP): overview and description of models, simulations and climate diagnostics (Lamarque et al., 2013b).

Evaluation of preindustrial to present-day black carbon and its albedo forcing from Atmospheric Chemistry and Climate Model Intercomparison Project (ACCMIP) (Lee et al., 2013).

Radiative forcing of the direct aerosol effect from AeroCom Phase II simulations (Myhre et al., 2013).

Preindustrial to present-day changes in tropospheric hydroxyl radical and methane lifetime from the Atmospheric Chemistry and Climate Model Intercomparison Project (ACCMIP) (Naik et al., 2013).

Comparison of spheroidal carbonaceous particle (SCP) data with modelled atmospheric black carbon concentration and deposition, and air mass sources in northern Europe, 1850-2010 (Ruppel et al., 2013).

Black carbon vertical profiles strongly affect its radiative forcing uncertainty (Samset et al., 2013).

Radiative forcing in the ACCMIP historical and future climate simulations (Shindell et al., 2013).

Global premature mortality due to anthropogenic outdoor air pollution and the contribution of past climate change (Silva et al., 2013).

Tropospheric ozone changes, radiative forcing and attribution to emissions in the Atmospheric Chemistry and Climate Model Intercomparison Project (ACCMIP) (Stevenson et al., 2013).

Analysis of present day and future OH and methane lifetime in the ACCMIP simulations (Voulgarakis et al., 2013).

Pre-industrial to end 21st century projections of tropospheric ozone from the Atmospheric Chemistry and Climate Model Intercomparison Project (ACCMIP) (Young et al., 2013).

K.6 2012 – 8 papers

Future air quality in Europe: a multi-model assessment of projected exposure to ozone (Colette et al., 2012).

Global air quality and climate (Fiore et al., 2012).

Future impact of traffic emissions on atmospheric ozone and OH based on two scenarios (Hodnebrog et al., 2012).

Attribution of the Arctic ozone column deficit in March 2011 (Isaksen et al., 2012).

Application of the CALIOP Layer Product to evaluate the vertical distribution of aerosols estimated by global models: Part 1. AeroCom phase I results (Koffi et al., 2012).

Parameterization of black carbon aging in the OsloCTM2 and implications for regional transport to the Arctic (Lund and Berntsen, 2012).

The chemical transport model Oslo CTM3 (Søvde et al., 2012).

Short-lived climate forcers from current shipping and petroleum activities in the Arctic (Ødemark et al., 2012).

K.7 2011 – 16 papers

Inferring absorbing organic carbon content from AERONET data (Arola et al., 2011).

Observed and Modelled record ozone decline over the Arctic during winter/spring 2011 (Balis et al., 2011).

Air quality trends in Europe over the past decade: a first multi-model assessment (Colette et al., 2011).

A note on the comparison between total ozone from Oslo CTM2 and SBUV satellite data (Eleftheratos et al., 2011).

Future impact of non-land based traffic emissions on atmospheric ozone and OH - an optimistic scenario and a possible mitigation strategy (Hodnebrog et al., 2011).

A review of the anthropogenic influence on biogenic secondary organic aerosol (Hoyle et al., 2011a).

Representation of tropical deep convection in atmospheric models - Part 2: Tracer transport (Hoyle et al., 2011b).

Global dust model intercomparison in AeroCom phase I (Huneus et al., 2011).

Strong atmospheric chemistry feedback to climate warming from Arctic methane emissions (Isaksen et al., 2011).

Radiative forcing due to changes in ozone and methane caused by the transport sector (Myhre et al., 2011).

Representation of tropical deep convection in atmospheric models - Part 1: Meteorology and comparison with satellite observations (Russo et al., 2011).

Vertical dependence of black carbon, sulphate and biomass burning aerosol radiative forcing (Samset and Myhre, 2011).

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The HNO₃ forming branch of the HO₂ + NO reaction: pre-industrial-to-present trends in atmospheric species and radiative forcings (Søvde et al., 2011a).

Estimation of Arctic Ozone Loss in the Winter 2006/07 using a Chemical Transport Model and Data Assimilation (Søvde et al., 2011b).

K.8 2010 – 4 papers

Direct radiative effect of aerosols emitted by transport: from road, shipping and aviation (Balkanski et al., 2010).

Impacts of the Large Increase in International Ship Traffic 2000-2007 on Tropospheric Ozone and Methane (Dalsøren et al., 2010).

Transport impacts on atmosphere and climate: Aviation (Lee et al., 2010).

Transport impacts on atmosphere and climate: Land transport (Uherek et al., 2010).

K.9 2009 – 13 papers

Effect of emission changes in southeast Asia on global hydroxyl and methane levels (Dalsøren et al., 2009b).

Update on emissions and environmental impacts from the international fleet of ships: the contribution from major ship types and ports (Dalsøren et al., 2009a).

Transport impacts on atmosphere and climate: Shipping (Eyring et al., 2009).

The impact of traffic emissions on atmospheric ozone and OH: results from QUANTIFY (Hoor et al., 2009).

Anthropogenic influence on SOA and the resulting radiative forcing (Hoyle et al., 2009a).

Present-day contribution of anthropogenic emissions

from China to the global burden and radiative forcing of aerosol and ozone (Hoyle et al., 2009b).

Atmospheric composition change: Climate-Chemistry interactions (Isaksen et al., 2009).

Evaluation of black carbon estimations in global aerosol models (Koch et al., 2009).

Modelled radiative forcing of the direct aerosol effect with multi-observation evaluation (Myhre et al., 2009b).

Consistency Between Satellite-Derived and Modeled Estimates of the Direct Aerosol Effect (Myhre, 2009).

Modelling of chemical and physical aerosol properties during the ADRIEX aerosol campaign (Myhre et al., 2009a).

The influence of foreign vs. North American emissions on surface ozone in the US (Reidmiller et al., 2009).

Costs and global impacts of black carbon abatement strategies (Rypdal et al., 2009).

K.10 2008 – 4 papers

Climate forcing from the transport sectors (Fuglestad et al., 2009).

Modeling of the solar radiative impact of biomass burning aerosols during the Dust and Biomass burning Experiment (DABEX) (Myhre et al., 2008).

European surface ozone in the extreme summer 2003 (Solberg et al., 2008).

Evaluation of the chemical transport model Oslo CTM2 with focus on Arctic winter ozone depletion (Søvde et al., 2008).

K.11 2007 – 10 papers

Sulphate trends in Europe: are we able to model the recent observed decrease? (Berglen et al., 2007).

Environmental impacts of the expected increase in sea transportation, with a particular focus on oil and gas scenarios for Norway and Northwest Russia (Dalsøren et al., 2007).

Changes in Nitrogen Dioxide and Ozone over South-east and East Asia between Year 2000 and 2030 with Fixed Meteorology (Gauss et al., 2007).

Climate impact of supersonic air traffic: An approach to optimize a potential future supersonic fleet - Results from the EU-project SCENIC (Grewe et al., 2007).

Secondary organic aerosol in the global aerosol -

chemical transport model Oslo CTM2 (Hoyle et al., 2007).

A Study of Tropospheric Ozone over China with a 3-D Global CTM Model (Liu et al., 2007).

Comparison of the radiative properties and direct radiative effect of aerosols from a global aerosol model and remote sensing data over ocean (Myhre et al., 2007a).

Aerosol-cloud interaction inferred from MODIS satellite data and global aerosol models (Myhre et al., 2007b).

Aircraft pollution: A futuristic view (Søvde et al., 2007).

The effect of harmonized emissions on aerosol properties in global models - an AeroCom experiment (Textor et al., 2007).

K.12 2006 – 13 papers

Abatement of Greenhouse Gases: Does Location Matter? (Berntsen et al., 2006).

CTM study of changes in tropospheric hydroxyl distribution 1990-2001 and its impact on methane (Dalsøren and Isaksen, 2006).

Nitrogen and sulfur deposition on regional and global scales: A multimodel evaluation (Dentener et al., 2006a).

The Global Atmospheric Environment for the Next Generation (Dentener et al., 2006b).

Impact of aircraft NOx emissions on the atmosphere - tradeoffs to reduce the impact (Gauss et al., 2006a).

Radiative forcing since preindustrial times due to ozone change in the troposphere and the lower stratosphere (Gauss et al., 2006b).

An AeroCom initial assessment - optical properties in aerosol component modules of global models (Kinne et al., 2006).

Modelling of nitrate and ammonium-containing aerosols in presence of sea salt (Myhre et al., 2006).

Multi-model ensemble simulations of tropospheric NO2 compared with GOME retrievals for the year 2000 (van Noije et al., 2006).

Radiative forcing by aerosols as derived from the AeroCom present-day and pre-industrial simulations (Schulz et al., 2006).

Multimodel simulations of carbon monoxide: Comparison with observations and projected near-future changes (Shindell et al., 2006).

Multimodel ensemble simulations of present-day and

near-future tropospheric ozone (Stevenson et al., 2006).

Analysis and quantification of the diversities of aerosol life cycles within AeroCom (Textor et al., 2006).

K.13 2005 – 5 papers

Response of climate to regional emissions of ozone precursors: sensitivities and warming potentials (Berntsen et al., 2005).

An evaluation of the performance of chemistry transport models - Part 2: Detailed comparison with two selected campaigns (Brunner et al., 2005).

Model simulations of dust sources and transport in the global atmosphere: Effects of soil erodibility and wind speed variability (Grini et al., 2005).

Tropospheric ozone changes at unpolluted and semipolluted regions induced by stratospheric ozone changes (Isaksen et al., 2005).

Radiative effect of surface albedo change from biomass burning (Myhre et al., 2005).

K.14 2004 – 4 papers

A global model of the coupled sulfur/oxidant chemistry in the troposphere: The sulfur cycle (Berglen et al., 2004).

Roles of saltation, sandblasting, and wind speed variability on mineral dust aerosol size distribution during the Puerto Rican Dust Experiment (PRIDE) (Grini and Zender, 2004).

NO_x change over China and its influences (Liu et al., 2004).

Uncertainties in the Radiative Forcing Due to Sulfate Aerosols (Myhre et al., 2004).

K.15 2003 – 10 papers

An evaluation of the performance of chemistry transport models by comparison with research aircraft observations. Part 1: Concepts and overall model performance (Brunner et al., 2003).

Emission from international sea transportation and environmental impact (Endresen et al., 2003).

Impact of H₂O emissions from cryoplanes and kerosene aircraft on the atmosphere (Gauss et al., 2003a).

Radiative forcing in the 21st century due to ozone

changes in the troposphere and the lower stratosphere (Gauss et al., 2003b).

Impact of aircraft NO_x emission on NO_x and ozone over China (Liu et al., 2003a).

The possible influences of the increasing anthropogenic emissions in India on tropospheric ozone and OH (Liu et al., 2003b).

Modeling the radiative impact of mineral dust during the Saharan Dust Experiment (SHADE) campaign (Myhre et al., 2003b).

Modeling the solar radiative impact of aerosols from biomass burning during the Southern African Regional Science Initiative (SAFARI-2000) experiment (Myhre et al., 2003a).

Fresh air in the 21st century? (Prather et al., 2003).

Chemical transport model ozone simulations for spring 2001 over the western Pacific: Comparisons with TRACE-P lidar, ozonesondes, and Total Ozone Mapping Spectrometer columns (Wild et al., 2003).

K.16 2002 – 4 papers

Modeling the Annual Cycle of Sea Salt in the Global 3D Model Oslo CTM2: Concentrations, Fluxes, and Radiative Impact (Grini et al., 2002).

Impacts of NO_x emissions from subsonic aircraft in a global three-dimensional chemistry transport model including plume processes (Kraabøl et al., 2002).

Model intercomparison of the transport of aircraft-like emissions from sub- and supersonic aircraft (Rogers et al., 2002).

Photochemical Activity and Solar Ultraviolet Radiation (PAUR) Modulation Factors: An overview of the project (Zerefos et al., 2002).

K.17 2001 – 4 papers

Atmospheric degradation and global warming potentials of three perfluoroalkenes (Acerboni et al., 2001).

Chemistry-transport model comparison with ozone observations in the midlatitude lowermost stratosphere (Bregman et al., 2001).

Model calculations of present and future levels of ozone and ozone precursors with a global and a regional model (Jonson et al., 2001).

Sulphate particles from subsonic aviation: impact on upper tropospheric and lower stratospheric ozone (Pitari et al., 2001).

K.18 Oslo CTM1 – 12 papers

NO_x Emissions from Aircraft: Its Impact on the Global Distribution of CH₄ and O₃ and on Radiative Forcing (Isaksen et al., 2001).

Time evolution of tropospheric ozone and its radiative forcing (Berntsen et al., 2000).

Trend analysis of O₃ and CO in the period 1980–1996: A three-dimensional model study (Karlsdóttir et al., 2000).

Radiative forcing due to changes in tropospheric ozone in the period 1980 to 1996 (Myhre et al., 2000).

Effects of lightning and convection on changes in tropospheric ozone due to NO_x emissions from aircraft (Berntsen et al., 1999).

Influence of Asian emissions on the composition of air reaching the north western United States (Berntsen et al., 1999).

3-D global simulations of tropospheric CO distributions: Results of the GIM/IGAC intercomparison 1997 exercise (Kanakidou et al., 1999).

Estimation of the direct radiative forcing due to sulfate and soot aerosols (Myhre et al., 1998).

Global distribution of sulphate in the troposphere: A three-dimensional model study (Restad et al., 1998).

Effects of anthropogenic emissions on tropospheric ozone and its radiative forcing (Berntsen et al., 1997).

A global three-dimensional chemical transport model: 2. Nitrogen oxides and nonmethane hydrocarbon results (Jaffe et al., 1997).

A global three-dimensional chemical transport model for the troposphere: 1. Model description and CO and Ozone results (Berntsen and Isaksen, 1997).

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Table 32: Oslo CTM3 v1.0 wet deposition parameters (Haslerud August 2017).

| Tracer | SOLU | CHN | TCHENA | TCHENB | TCKAQA | TCKAQB | ISCVFR | IT |
|----------|------|-----|---------|--------|--------|--------|---------|----|
| O3 | 1.00 | 1 | 1.1d-02 | 2400 | 0 | 0 | 0.0d-00 | 0 |
| OH | 1.00 | 0 | 2.5d+01 | 5300 | 0 | 0 | 0.0d-00 | 0 |
| HO2 | 1.00 | 1 | 4.0d+03 | 5900 | 0 | 0 | 0.0d-00 | 0 |
| NO | 1.00 | 0 | 1.9d-03 | 1400 | 0 | 0 | 0.0d-00 | 0 |
| NO3 | 1.00 | 1 | 2.0d+00 | 2000 | 0 | 0 | 0.0d-00 | 0 |
| NO2 | 1.00 | 0 | 1.2d-02 | 2500 | 0 | 0 | 0.0d-00 | 0 |
| N2O5 | 1.00 | 1 | 2.1d+00 | 3400 | 0 | 0 | 0.0d-00 | 0 |
| HONO | 1.00 | 0 | 4.9d+01 | 4800 | 0 | 0 | 0.0d-00 | 0 |
| HN03 | 1.00 | 3 | 2.1d+05 | 8700 | 1 | 1 | 1.0d-00 | 1 |
| HO2NO2 | 1.00 | 1 | 1.2d+04 | 6900 | 0 | 0 | 0.0d-00 | 0 |
| H2O2 | 1.00 | 1 | 7.1d+04 | 6800 | 0 | 1 | 0.0d-00 | 0 |
| CH4 | 1.00 | 0 | 1.4d-03 | 1600 | 0 | 0 | 0.0d-00 | 0 |
| CH3O2 | 1.00 | 1 | 2.0d+03 | 6600 | 0 | 0 | 0.0d-00 | 0 |
| CH3O2H | 1.00 | 1 | 3.1d+02 | 5200 | 0 | 0 | 0.0d-00 | 0 |
| CH2O | 1.00 | 1 | 3.2d+03 | 6800 | 1 | 0 | 0.0d-00 | 0 |
| CO | 1.00 | 0 | 9.5d-04 | 1300 | 0 | 0 | 0.0d-00 | 0 |
| O2 | 1.00 | 0 | 1.3d-03 | 1500 | 0 | 0 | 0.0d-00 | 0 |
| N2 | 1.00 | 0 | 6.1d-04 | 1300 | 0 | 0 | 0.0d-00 | 0 |
| C2H6 | 1.00 | 0 | 1.9d-03 | 2300 | 0 | 0 | 0.0d-00 | 0 |
| C2H5O2 | 1.00 | 1 | 2.2d+03 | 7200 | 0 | 0 | 0.0d-00 | 0 |
| EtOOH | 1.00 | 0 | 3.4d+02 | 6000 | 0 | 0 | 0.0d-00 | 0 |
| CH3CHO | 1.00 | 1 | 1.4d+01 | 5600 | 0 | 0 | 0.0d-00 | 0 |
| MeCO3 | 1.00 | 0 | 1.0d-01 | 0 | 0 | 0 | 0.0d-00 | 0 |
| PANX | 1.00 | 1 | 2.9d+00 | 5900 | 0 | 0 | 0.0d-00 | 0 |
| Alkane | 1.00 | 0 | 1.2d-03 | 3100 | 0 | 0 | 0.0d-00 | 0 |
| ROH00 | 1.00 | 0 | 0.0d+00 | 0 | 0 | 0 | 0.0d-00 | 0 |
| Alkene | 1.00 | 0 | 7.4d-03 | 3400 | 0 | 0 | 0.0d-00 | 0 |
| Aromatic | 1.00 | 0 | 1.5d-01 | 4000 | 0 | 0 | 0.0d-00 | 0 |
| ISOPRENE | 1.00 | 0 | 1.3d-02 | 0 | 0 | 0 | 0.0d-00 | 0 |
| MVKMACR | 1.00 | 0 | 2.1d+01 | 7800 | 0 | 0 | 0.0d-00 | 0 |
| ISOK | 1.00 | 1 | 1.3d+01 | 7800 | 0 | 0 | 0.0d-00 | 0 |
| H2S | 1.00 | 0 | 8.7d-02 | 2100 | 0 | 0 | 0.0d-00 | 0 |
| DMS | 1.00 | 0 | 4.8d-01 | 3100 | 0 | 0 | 0.0d-00 | 0 |
| Me2SO | 1.00 | 0 | 5.0d+04 | 0 | 0 | 0 | 0.0d-00 | 0 |
| Me2SO2 | 1.00 | 0 | 5.0d+04 | 0 | 0 | 0 | 0.0d-00 | 0 |
| MeSO3H | 1.00 | 0 | 1.0d+08 | 0 | 0 | 0 | 0.0d-00 | 0 |
| MSA | 1.00 | 3 | 5.0d+04 | 0 | 0 | 0 | 0.0d-00 | 0 |
| SO2 | 1.00 | 1 | 1.2d+00 | 3020 | 1 | 0 | 0.0d-00 | 0 |
| SO3 | 1.00 | 0 | 1.0d+08 | 0 | 0 | 0 | 0.0d-00 | 0 |
| SO4 | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.1d-00 | 0 |
| SF6 | 1.00 | 0 | 2.4d-04 | 2400 | 0 | 0 | 0.0d-00 | 0 |
| Rn | 1.00 | 0 | 9.3d-03 | 2600 | 0 | 0 | 0.0d-00 | 0 |
| omBB1fil | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.1d-00 | 4 |
| omFF1fil | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.1d-00 | 4 |
| omBF1fil | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.1d-00 | 4 |
| omOCNfil | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.1d-00 | 4 |
| omBB1fob | 1.00 | 6 | 1.0d+08 | 0 | 0 | 1 | 0.2d-00 | 4 |
| omFF1fob | 1.00 | 6 | 1.0d+08 | 0 | 0 | 1 | 0.2d-00 | 4 |
| omBF1fob | 1.00 | 6 | 1.0d+08 | 0 | 0 | 1 | 0.2d-00 | 4 |
| omOCNfob | 1.00 | 6 | 1.0d+08 | 0 | 0 | 1 | 0.2d-00 | 4 |
| bcBB1fil | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.1d-00 | 4 |
| bcFF1fil | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.1d-00 | 4 |
| bcBF1fil | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.1d-00 | 4 |
| bcBB1fob | 1.00 | 6 | 1.0d+08 | 0 | 0 | 1 | 0.2d-00 | 4 |
| bcFF1fob | 1.00 | 6 | 1.0d+08 | 0 | 0 | 1 | 0.2d-00 | 4 |
| bcBF1fob | 1.00 | 6 | 1.0d+08 | 0 | 0 | 1 | 0.2d-00 | 4 |

Table 33: Oslo CTM3 v1.0 wet deposition parameters continued for sea salt, mineral dust and nitrate.

| Tracer | SOLU | CHN | TCHENA | TCHENB | TCKAQA | TCKAQB | ISCVFR | IT |
|-----------|------|-----|---------|--------|--------|--------|---------|----|
| SALT01 | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.1d-00 | 0 |
| SALT02 | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.1d-00 | 0 |
| SALT03 | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.1d-00 | 0 |
| SALT04 | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.1d-00 | 0 |
| SALT05 | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.1d-00 | 0 |
| SALT06 | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.1d-00 | 0 |
| SALT07 | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.1d-00 | 0 |
| SALT08 | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.1d-00 | 0 |
| DUST01 | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.5d-00 | 4 |
| DUST02 | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.5d-00 | 4 |
| DUST03 | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.5d-00 | 4 |
| DUST04 | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.5d-00 | 4 |
| DUST05 | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.5d-00 | 4 |
| DUST06 | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.5d-00 | 4 |
| DUST07 | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.5d-00 | 4 |
| DUST08 | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.5d-00 | 4 |
| HN03s | 1.00 | 3 | 2.1d+05 | 8700 | 1 | 1 | 1.0d-00 | 1 |
| NH3 | 1.00 | 1 | 3.3d+06 | 0 | 0 | 0 | 0.0d-00 | 0 |
| NH4fine | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.1d-00 | 0 |
| NH4coarse | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.1d-00 | 0 |
| N03fine | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.1d-00 | 0 |
| N03coarse | 1.00 | 3 | 1.0d+08 | 0 | 0 | 1 | 0.1d-00 | 0 |

Table 34: Oslo CTM3 v1.0 wet deposition parameters continued for SOA species.

| Tracer | SOLU | CHN | TCHENA | TCHENB | TCKAQA | TCKAQB | ISCVFR | IT |
|----------|------|-----|---------|--------|--------|--------|---------|----|
| SOAGAS11 | 1.00 | 1 | 1.0d+05 | 12 | 0 | 0 | 1.0d-00 | 0 |
| SOAGAS21 | 1.00 | 1 | 1.0d+05 | 12 | 0 | 0 | 1.0d-00 | 0 |
| SOAGAS31 | 1.00 | 1 | 1.0d+05 | 12 | 0 | 0 | 1.0d-00 | 0 |
| SOAGAS41 | 1.00 | 1 | 1.0d+05 | 12 | 0 | 0 | 1.0d-00 | 0 |
| SOAGAS51 | 1.00 | 1 | 1.0d+05 | 12 | 0 | 0 | 1.0d-00 | 0 |
| SOAGAS12 | 1.00 | 1 | 1.0d+05 | 12 | 0 | 0 | 1.0d-00 | 0 |
| SOAGAS22 | 1.00 | 1 | 1.0d+05 | 12 | 0 | 0 | 1.0d-00 | 0 |
| SOAGAS32 | 1.00 | 1 | 1.0d+05 | 12 | 0 | 0 | 1.0d-00 | 0 |
| SOAGAS42 | 1.00 | 1 | 1.0d+05 | 12 | 0 | 0 | 1.0d-00 | 0 |
| SOAGAS52 | 1.00 | 1 | 1.0d+05 | 12 | 0 | 0 | 1.0d-00 | 0 |
| SOAGAS13 | 1.00 | 1 | 1.0d+05 | 12 | 0 | 0 | 1.0d-00 | 0 |
| SOAGAS23 | 1.00 | 1 | 1.0d+05 | 12 | 0 | 0 | 1.0d-00 | 0 |
| SOAGAS33 | 1.00 | 1 | 1.0d+05 | 12 | 0 | 0 | 1.0d-00 | 0 |
| SOAGAS43 | 1.00 | 1 | 1.0d+05 | 12 | 0 | 0 | 1.0d-00 | 0 |
| SOAGAS53 | 1.00 | 1 | 1.0d+05 | 12 | 0 | 0 | 1.0d-00 | 0 |
| SOAGAS61 | 1.00 | 1 | 1.0d+05 | 12 | 0 | 0 | 1.0d-00 | 0 |
| SOAGAS62 | 1.00 | 1 | 1.0d+05 | 12 | 0 | 0 | 1.0d-00 | 0 |
| SOAGAS71 | 1.00 | 1 | 1.0d+04 | 12 | 0 | 0 | 1.0d-00 | 0 |
| SOAGAS72 | 1.00 | 1 | 1.0d+03 | 12 | 0 | 0 | 1.0d-00 | 0 |
| SOAGAS81 | 1.00 | 1 | 1.0d+03 | 12 | 0 | 0 | 1.0d-00 | 0 |
| SOAGAS82 | 1.00 | 1 | 1.0d+03 | 12 | 0 | 0 | 1.0d-00 | 0 |
| Apine | 1.00 | 1 | 2.3d-02 | 0 | 0 | 0 | 1.0d-00 | 0 |
| Bpine | 1.00 | 1 | 2.3d-02 | 0 | 0 | 0 | 1.0d-00 | 0 |
| Sabine | 1.00 | 1 | 2.3d-02 | 0 | 0 | 0 | 1.0d-00 | 0 |
| D3carene | 1.00 | 1 | 2.3d-02 | 0 | 0 | 0 | 1.0d-00 | 0 |
| Trp_Ket | 1.00 | 1 | 2.3d-02 | 0 | 0 | 0 | 1.0d-00 | 0 |
| Limon | 1.00 | 1 | 7.0d-02 | 0 | 0 | 0 | 1.0d-00 | 0 |
| Trpolene | 1.00 | 1 | 6.7d-02 | 0 | 0 | 0 | 1.0d-00 | 0 |
| Trpinene | 1.00 | 1 | 6.7d-02 | 0 | 0 | 0 | 1.0d-00 | 0 |
| Myrcene | 1.00 | 1 | 5.4d+01 | 0 | 0 | 0 | 1.0d-00 | 0 |
| Ocimene | 1.00 | 1 | 5.4d+01 | 0 | 0 | 0 | 1.0d-00 | 0 |
| TrpAlc | 1.00 | 1 | 5.4d+01 | 0 | 0 | 0 | 1.0d-00 | 0 |
| Sestrp | 1.00 | 1 | 4.9d-02 | 0 | 0 | 0 | 1.0d-00 | 0 |
| SOAAER11 | 0.80 | 3 | 1.0d+08 | 0 | 0 | 1 | 2.0d-01 | 4 |
| SOAAER21 | 0.80 | 3 | 1.0d+08 | 0 | 0 | 1 | 2.0d-01 | 4 |
| SOAAER31 | 0.80 | 3 | 1.0d+08 | 0 | 0 | 1 | 2.0d-01 | 4 |
| SOAAER41 | 0.80 | 3 | 1.0d+08 | 0 | 0 | 1 | 2.0d-01 | 4 |
| SOAAER51 | 0.80 | 3 | 1.0d+08 | 0 | 0 | 1 | 2.0d-01 | 4 |
| SOAAER12 | 0.80 | 3 | 1.0d+08 | 0 | 0 | 1 | 2.0d-01 | 4 |
| SOAAER22 | 0.80 | 3 | 1.0d+08 | 0 | 0 | 1 | 2.0d-01 | 4 |
| SOAAER32 | 0.80 | 3 | 1.0d+08 | 0 | 0 | 1 | 2.0d-01 | 4 |
| SOAAER42 | 0.80 | 3 | 1.0d+08 | 0 | 0 | 1 | 2.0d-01 | 4 |
| SOAAER52 | 0.80 | 3 | 1.0d+08 | 0 | 0 | 1 | 2.0d-01 | 4 |
| SOAAER13 | 0.80 | 3 | 1.0d+08 | 0 | 0 | 1 | 2.0d-01 | 4 |
| SOAAER23 | 0.80 | 3 | 1.0d+08 | 0 | 0 | 1 | 2.0d-01 | 4 |
| SOAAER33 | 0.80 | 3 | 1.0d+08 | 0 | 0 | 1 | 2.0d-01 | 4 |
| SOAAER43 | 0.80 | 3 | 1.0d+08 | 0 | 0 | 1 | 2.0d-01 | 4 |
| SOAAER53 | 0.80 | 3 | 1.0d+08 | 0 | 0 | 1 | 2.0d-01 | 4 |
| SOAAER61 | 0.80 | 3 | 1.0d+08 | 0 | 0 | 1 | 2.0d-01 | 4 |
| SOAAER62 | 0.80 | 3 | 1.0d+08 | 0 | 0 | 1 | 2.0d-01 | 4 |
| SOAAER71 | 0.80 | 3 | 1.0d+08 | 0 | 0 | 1 | 2.0d-01 | 4 |
| SOAAER72 | 0.80 | 3 | 1.0d+08 | 0 | 0 | 1 | 2.0d-01 | 4 |
| SOAAER81 | 0.80 | 3 | 1.0d+08 | 0 | 0 | 1 | 2.0d-01 | 4 |
| SOAAER82 | 0.80 | 3 | 1.0d+08 | 0 | 0 | 1 | 2.0d-01 | 4 |

Table 35: ECMWF meteorological fields in netCDF4 files and in UiO binary files. Units, whether field is instantaneous or accumulated (I/A). If field is used in Oslo CTM3, it has a CTM name. Also lists the UiO index and file where data is found: spectral (SP), gridded 3D (GG) or gridded 2D (surface, SFC).

| Field name | CTM name | Description | Unit | I/A | UiO ID | UiO file |
|---|--------------------|---|---|-----|--------|----------|
| lon | XDGRD [†] | Longitude at grid center | degree East | — | — | — |
| lat | YDGRD [†] | Latitude at grid center | degree North | — | — | — |
| ilon | XDEDG [†] | Longitude at interstices | degree East | — | — | — |
| ilat | YDEDG [†] | Latitude at interstices | degree North | — | — | — |
| hyai | ETAA [†] | Hybrid sigma coordinate A at interstices | hPa | — | — | — |
| hybi | ETAB [†] | Hybrid sigma coordinate B at interstices | 0–1 | — | — | — |
| data_date | — | Date and UTC hour for data given as YYYYMMDDHH | — | — | — | — |
| time_span | — | Time span of accumulated period i.e. meteorological time step | s | — | — | — |
| [†] Field is not read, but is calculated or read from other input. | | | | | | |
| temperature | T | Temperature | K | I | 130 | SPE |
| U | U | Horizontal wind at grid center* Unit is converted in CTM: | m/s*cos(lat) kg/s | I | — | — |
| V | V | Meridional wind at interstices* Unit is converted in CTM: | m/s*cos(lat) kg/s | I | — | — |
| *In UiO format, U and V are calculated from vorticity and divergence: | | | | | | |
| | | Vorticity, relative* | s ⁻¹ | I | 138 | SPE |
| | | Divergence* | s ⁻¹ | I | 155 | SPE |
| qhum | Q | Specific humidity | kg/kg | I | 133 | GG |
| lwc | CLDLWC | Cloud liquid water content | kg/kg | I | 246 | GG |
| iwc | CLDIWC | Cloud ice water content | kg/kg | I | 247 | GG |
| cfr | CLDFR | Cloud cover | (0–1) | I | 248 | GG |
| cfxu | — | Mass flux into updrafts (1/2-levels starting first level above sfc) | kg m ⁻² s ⁻¹ | A | 212 | GG |
| cfxd | CWETE | Unit is converted in CTM: | kg s ⁻¹ | | | |
| | — | Mass flux into downdrafts (1/2-levels starting first level above sfc) | kg m ⁻² s ⁻¹ | A | 213 | GG |
| cdetu | CWETD | Unit is converted in CTM: | kg s ⁻¹ | | | |
| | CDETU | Mass flux detrainment into updrafts | kg m ⁻³ s ⁻¹ | A | 214 | GG |
| cdetd | — | Unit is converted in CTM: | kg s ⁻¹ | | | |
| | CDETD | Mass flux detrainment into downdrafts | kg m ⁻³ s ⁻¹ | A | 215 | GG |
| convrain | — | Unit is converted in CTM: | kg s ⁻¹ | | | |
| | PRECCNV | Convective precipitation (half-levels starting at surface) | kg m ⁻² s ⁻¹ | A | 217 | GG |
| lsrain | — | Unit is converted in CTM: | kg s ⁻¹ | | | |
| | PRECLS | Large scale precipitation (half-levels starting at surface) | kg m ⁻² s ⁻¹ | A | 218 | GG |
| PV | — | Unit is converted in CTM: | kg s ⁻¹ | | | |
| | PVU | Potential Vorticity | K m ² kg ⁻¹ s ⁻¹ | I | 60 | GG |
| | | Unit is converted to PVU in CTM: | 10 ⁶ PV | | | |
| Some derived 3D fields in Oslo CTM3 | | | | | | |
| — | CENTU | Mass flux entrainment into updrafts | kg s ⁻¹ | | | |
| — | CENTD | Calculated from CWETE and CDETU. Mass flux entrainment into downdrafts | kg s ⁻¹ | | | |
| — | ZOFLE | Calculated from CWETD and CDETD. Height of grid box interstices (bottom) | m | | | |

Table 36: Meteorological fields (continued).

| Field name | CTM name | Description | Unit | I/A | UiO ID | UiO file |
|------------|----------|---|-----------------------------|-----|--------|----------|
| U10M | SFU | 10 metre U wind component | m s^{-1} | I | 165 | SFC |
| V10M | SFV | 10 metre V wind component | m s^{-1} | I | 166 | SFC |
| U10G | — | 10 metre wind gust | m s^{-1} | I | 49 | SFC |
| TDEW2M | — | 2 metre dewpoint temperature to calculate specific humidity SFQ | K | I | 168 | SFC |
| T2M | SFT | 2 metre temperature | K | I | 167 | SFC |
| BLD | — | Boundary layer dissipation | W m^{-2} | A | 145 | SFC |
| BLH | BLH_CUR | Boundary layer height for current time step | m | I | 159 | SFC |
| BLH | BLH_NEXT | Boundary layer height for next time step | m | I | 159 | SFC |
| | BLH | Boundary layer height Set from BLH_CUR and BLH_NEXT | m | I | 159 | SFC |
| CHNK | — | Charnock parameter | — | I | 148 | SFC |
| CAPE | — | Convective available potential energy | J kg^{-1} | I | 59 | SFC |
| CONVPREC | — | Convective precipitation | m | A | 143 | SFC |
| DUVRS | — | Downward UV radiation at the surface | W m^{-2} | A | 57 | SFC |
| EWSS | EWSS | East-West surface stress | N m^{-2} | A | 180 | SFC |
| E | — | Evaporation | m of water | A | 182 | SFC |
| SA | SA | Forecast surface albedo | 0–1 | I | 243 | SFC |
| FLZOH | — | Forecast $\ln(\text{surface roughness for heat})$ | $\ln(\text{m})$ | I | 245 | SFC |
| FSR | — | Forecast surface roughness | m | I | 244 | SFC |
| ZSFC | — | Surface Geopotential | $\text{m}^2 \text{s}^{-2}$ | I | 129 | SFC |
| GWD | — | Gravity wave dissipation | $\text{W m}^{-2} \text{ s}$ | A | 197 | SFC |
| HCC | — | High cloud cover | 0–1 | I | 188 | SFC |
| ISTL1 | — | Ice surface temperature layer 1 | K | I | 35 | SFC |
| ISTL2 | — | Ice surface temperature layer 2 | K | I | 36 | SFC |
| ISTL3 | — | Ice surface temperature layer 3 | K | I | 37 | SFC |
| ISTL4 | — | Ice surface temperature layer 4 | K | I | 38 | SFC |
| LSM | — | Land-sea mask | 0–1 | I | 172 | SFC |
| LSPF | — | Large-scale precipitation fraction | 0–1 | A | 50 | SFC |
| LSPREC | LSPREC | Large-scale precipitation | m | A | 142 | SFC |
| LGWS | — | Latitudinal component of gravity wave stress | N m^{-2} | A | 195 | SFC |
| LZOH | — | $\ln(\text{surface roughness length for heat})$ | $\ln(\text{m})$ | I | 234 | SFC |
| LCC | — | Low cloud cover | 0–1 | I | 186 | SFC |
| MX2T | — | Maximum temperature at 2 m | K | I | 201 | SFC |
| MSLP | — | Mean sea level pressure | Pa | I | 151 | SFC |
| MCC | — | Medium cloud cover | 0–1 | I | 187 | SFC |
| MGWS | — | Meridional component of gravity wave stress | N m^{-2} | A | 196 | SFC |
| MN2T | — | Minimum temperature at 2m | K | I | 202 | SFC |
| NSSS | NSSS | North-South surface stress | N m^{-2} | A | 181 | SFC |
| PAR | PAR | Photosynthetically active radiation at the surface | W m^{-2} | A | 58 | SFC |
| RO | — | Runoff | m | A | 205 | SFC |
| SSTK | — | Sea surface temperature-Kelvin | K | I | 34 | SFC |
| CI | CI | Sea-ice cover | 0–1 | I | 31 | SFC |
| SRC | — | Skin reservoir content | m of water | I | 198 | SFC |
| SKT | — | Skin temperature | K | I | 235 | SFC |
| ASN | — | Snow albedo | 0–1 | I | 32 | SFC |
| RSN | — | Snow density | kg m^{-3} | I | 33 | SFC |
| SD | SD | Snow depth | m of water equivalent | I | 141 | SFC |
| ES | ES | Snow evaporation | m of water equivalent | A | 44 | SFC |
| SF | SF | Snowfall (conv. + strat.) | m of water equivalent | A | 144 | SFC |
| SMLT | SMLT | Snowmelt | m of water | A | 45 | SFC |
| STL1 | — | Soil temperature level 1 | K | I | 139 | SFC |
| STL2 | — | Soil temperature level 2 | K | I | 170 | SFC |
| STL3 | — | Soil temperature level 3 | K | I | 183 | SFC |
| STL4 | — | Soil temperature level 4 | K | I | 236 | SFC |
| SUND | — | Sunshine duration | 1 | A | 189 | SFC |
| SLHF | SLH | Surface latent heat flux | W m^{-2} | A | 147 | SFC |

Table 37: Meteorological fields (continued).

| Field name | CTM name | Description | Unit | I/A | UiO ID | UiO file |
|---|----------|--|--------------------|-----|--------|----------|
| SNSRCS | — | Surface net solar radiation, clear sky | W m^{-2} | A | 210 | SFC |
| SNTRCS | — | Surface net thermal radiation, clear sky | W m^{-2} | A | 211 | SFC |
| pres_sfc | P | Surface pressure UiO format: ln(Pa) | hPa | I | 152 | SPE |
| SSHF | SHF | Surface sensible heat flux | W m^{-2} | A | 146 | SFC |
| SSR | — | Surface solar radiation | W m^{-2} | A | 176 | SFC |
| SSRD | SSRD** | Surface solar radiation downwards | W m^{-2} | A | 169 | SFC |
| STR | — | Surface thermal radiation | W m^{-2} | A | 177 | SFC |
| STRD | STRD** | Surface thermal radiation downwards | W m^{-2} | A | 177 | SFC |
| TSN | — | Temperature of snow layer | K | I | 238 | SFC |
| TSRC | — | Top net solar radiation, clear sky | W m^{-2} | A | 208 | SFC |
| TTRC | — | Top net thermal radiation, clear sky | W m^{-2} | A | 209 | SFC |
| TSR | — | Top solar radiation | W m^{-2} | A | 178 | SFC |
| TTR | — | Top thermal radiation | W m^{-2} | A | 179 | SFC |
| TCC | — | Total cloud cover | 0–1 | I | 164 | SFC |
| TCIW | — | Total column ice water | kg m^{-2} | I | 79 | SFC |
| TCLW | — | Total column liquid water | kg m^{-2} | I | 78 | SFC |
| TCW | — | Total column water | kg m^{-2} | I | 136 | SFC |
| TCWV | — | Total column water vapor | kg m^{-2} | I | 137 | SFC |
| SWVL1 | SWVL1** | Volumetric soil water layer 1 | m m^{-3} | I | 39 | SFC |
| SWVL2 | — | Volumetric soil water layer 2 | m m^{-3} | I | 40 | SFC |
| SWVL3 | — | Volumetric soil water layer 3 | m m^{-3} | I | 41 | SFC |
| SWVL4 | — | Volumetric soil water layer 4 | m m^{-3} | I | 42 | SFC |
| ** These are available only in DUST code. | | | | | | |
| Some derived 2D fields in Oslo CTM3 | | | | | | |
| — | SFQ | Specific humidity at surface | kg/kg | I | — | — |
| — | USTR | Friction velocity | m/s | I | — | — |

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