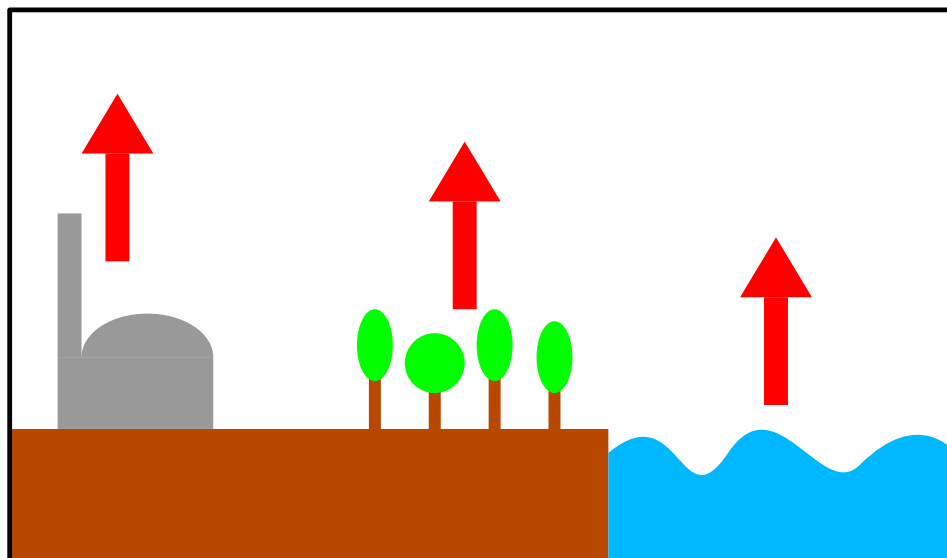# MESSy Emissions Users Manual

Astrid Kerkweg, Rolf Sander,
Holger Tost & Patrick Jöckel

for the MESSy submodels and tools:

OFFLEM: *offline calculated (prescribed) emissions*

EDGAR2NC: *emission pre-processor*

TNUDGE: *tracer nudging (pseudo-emissions)*

ONLEM: *online calculated emissions*

Air Chemistry Department
Max-Planck Institute of Chemistry
PO Box 3060, 55020 Mainz, Germany
`akerkweg@mpch-mainz.mpg.de`

Date: 2006/02/13

Contents

1   Introduction

We present the technical structure of the two emission submodels ONLEM and OFFLEM as well as the "pseudo-emission" submodel TNUDGE. All these submodels are part of MESSy (Jöckel et al., 2005). In addition, the conversion tool EDGAR2NC is introduced. These submodels and tools provide a very easy way of implementing new emissions into a model, which is much less prone to produce errors than conventional schemes.

Not every emission can be described by an offline emission field. Emissions depending on model variables have to be calculated online within the model, e.g., sea salt emissions which depend on the wind speed. The submodel ONLEM deals with these kinds of emissions. As far as possible it uses the same structure as OFFLEM. Only the calculation of the emission itself, which is done in OFFLEM fully automatically, is performed by one subroutine call for each emission *type*. Thus implementing a new online calculated emission is achieved by adding one new submodel core layer (SMCL) routine containing the physical substance of the emission (e.g. the wind dependent source function for sea salt emissions) and an additional entry into the ONLEM namelist file.

The following sections describe how the user can adjust the settings of the submodels using the entries in the Fortran90 namelist files. These files contain a control namelist (`&CTRL`), a coupling namelist (`&CPL`), and/or a namelist called `&RGTEVENTS` for triggering the regular update of time-dependent boundary conditions.

2   Prescribed Emissions (OFFLEM)

The namelist file begins with the coupling namelist `&CPL`. It contains two entries which affect the output of the submodel. The first switch `l_gp` determines whether emissions are calculated for grid point (GP) tracers. The

generic tracer submodel of MESSy (Jöckel, manuscript in preparation) provides the possibility to distinguish between different tracer sets (e.g., tracers in Lagrangian representation in addition to those in grid point representation). Setting the second switch `l_force` to `.TRUE.` forces the OFFLEM submodel to import also those fluxes for which tracers are not available.

The second part of the OFFLEM namelist file contains the individual emissions. As every emission is associated with an offline emission field that is read via the MESSy data import interface (Jöckel, 2006), the setup is not determined within a control namelist (`&CTRL`), but by a list of so-called regridding triggers. Each trigger is indicated by the keyword `RG_TRIG` and the number of the trigger in parentheses, e.g. `RG_TRIG(1)` followed by its definition such as:

`RG_TRIG(n)` = *event, stepper,*

where `n` is an arbitrary, but unambiguous number in a list of regridding triggers.

The *event* defines a periodically occuring event, e.g., for using different emissions every month. The event handler programmed by Ingo Kirchner is part of ECHAM5 and described in more detail in the NCREGRID documentation (see Jöckel, 2006).

An *event* consists of four comma-separated entries:

event = interval, unit, adjustment, offset

interval is an integer describing the trigger time interval in the given *unit*, which is one of `'seconds'`, `'minutes'`, `'days'`, `'months'`, `'years'` or `'steps'`, where `'steps'` refers to the length of one model time step. *adjustment* is a string for adjustment inside the unit (The keywords `'first'` and `'last'` trigger the event at the first or at the last model time step within the given *interval*, respectively. No adjustment takes place when the keyword `'exact'` is given, i.e. the event is triggered exactly at the model start date and then every `interval`). *offset* is an integer for the offset to the initial date (in seconds). For example, the entry `1,'months','first',0` which is shown in in Fig. 1 indicates that the event triggers at the beginning of every (`1`) month as determined by the keywords `'first'` and `'months'`. The fourth entry (`0`) indicates that the event is triggerd at the beginning of the first month i.e., without any offset.

The *stepper* consists of a *counter* and the *action string*. The *counter* is defined as:

counter = name, min, step, max, start

It defines the cyclic stepping through the time steps of the netCDF input file. *name* is a string defining a name by which the *counter* can be identified. *start* is the initial value of the *counter* at the very first model time step. During the simulation the *counter* is increased by *step* until *max* is reached. Afterwards the *counter* is reset to *min*. In the example in Fig. 1, the *counter* with the name `'n003'` starts with 13, is incremented by 1 at the beginning of

```
&CPL
l_gp      = T  ! emissions for gridpoint tracers
l_force   = T  ! force import of data set even if tracer is not present
/

&RGTEVENTS
!               [------ event -----], [-------------------------- stepper -------------------------]
!                                     [--- counter ----], [------------- action string --------------]
RG_TRIG(3)  = 1,'months','first',0, 'n003', 73,1,84,13, 'GP=0; NML=./offlem/sfmr_CFC.nml; VAR=CFCl3'
RG_TRIG(4)  = 1,'months','first',0, 'n004', 73,1,84,13, 'GP=0; NML=./offlem/sfmr_CFC.nml; VAR=CF2Cl2'
RG_TRIG(27) = 1,'months','first',0,       , 1,1,12,1,  'GP=1; NML=./offlem/emis_NH3.nml; VAR=NH3;'
RG_TRIG(26) = 1,'months','first',0,       , 1,1,12,1,  'GP=1; NML=./offlem/so2_2000.nml; VAR=SO2;
                                                          Z=45,140,240,400,600,800'
RG_TRIG(25) = 1,'months','first',0,       , 1,1,12,1,  'GP=1; NML=./offlem/emis_airc_NOx_1995.nml'
RG_TRIG(30) = 1,'months','first',0,       , 1,1,12,1,  'GP=2; NML=./offlem/emis_CH3I.nml;
                                                          FILE=/data/emissions/emis_CH3I.nc'
/
```

Figure 1: Example for an OFFLEM namelist file showing every possible combination of emission *types* and emission *methods*. Triggers 3 and 4 show examples for files which are only read by OFFLEM (GP=0). Trigger 27 defines a surface emission (2D), 26 is a multilayer 2D emission (Nx2D), and 25 is a volume emission (3D). These three emissions are directly assigned to the respective tracers tendency (GP=1). Finally, trigger 30 is an example for a 2D emission from which a lower boundary condition for the diffusive flux is calculated (GP=2). Additionally the location of the CH_3I emission file is explicitly named in this example.

each month until 84 is reached, then the *counter* is reset to 73.

Finally, the *action string* controls submodel-specific features. In the OFFLEM stepper action string the following keywords, separated by semicolons, are recognized:

- GP= followed by 0, 1 or 2, defines the emission *method* for the corresponding grid point (GP) tracer. One of the three emission methods must be given: 0 (default) for storage in memory only, 1 indicating tracer tendency calculation, and 2 for the modification of the lower flux boundary condition.

- NML= followed by the name (including the path) of the file containing the namelist for NCREGRID. If this keyword is omitted (or empty), the OFFLEM namelist file itself (offlem.nml) is used as NCREGRID namelist file.

- FILE= followed by the name (including the path) of the emission data file. NCREGRID loops over all NCREGRID namelists in the specific namelist file (the result of NML=), until the first namelist with matching netCDF-filename is found. If this keyword is omitted (or empty), the first namelist in the specified namelist file (the result of NML=) is used.

- VAR= followed by the name of the variable that is imported by NCREGRID. NCREGRID loops over all NCREGRID namelists in a specific namelist file (the result of NML=), until the first namelist with matching variable name is found (in this case, the

FILE specifier is ignored). If this keyword is omitted, NCREGRID imports all variables from FILE, if specified, or all variables from the first NCREGRID namelist in NML.

- Z= followed by a comma-separated list of geometric emission heights (in meter above ground). This is only applicable to multilevel (Nx2D) emissions. The number of emission heights must match the number of emission levels (N) in the input file.

The tracer(s) corresponding to a specific emission is/are determined by the name of the imported variable(s), i.e., either specified by the keyword VAR=, or by the NCRE-GRID namelist from the input file. The summation of different contributions (spread over multiple netCDF files) as emission into one tracer can be achieved by using the FILE= or VAR= specifier in combination with the NML= specifier.

For volume emissions (3D), the corresponding NCRE-GRID namelist must contain the specification of the vertical coordinate, and the Z= specifier (emission heights) must not be used. In contrast to this, the presence of the Z= specifier (emission heights) in the stepper action string is the keyword for multilevel emissions (Nx2D). In this case, the corresponding NCREGRID-namelist must not contain any specification of a vertical coordinate, since the levels must be treated as an 'invariant' (parameter-) dimension. Furthermore, for Nx2D emissions, the FILE= specifier must not be used, since for Nx2D the level must be treated by NCREGRID as invariant dimension. Re-gridding of a file (i.e., multiple variables in one step) containing one or more variables with a free parameter (here

```
&CTRL
OUTPUT       = 'example.nc'
SPECIES      = 'N2O'
L_MASSFLUX   = F
MOLARMASS    = 44.02
YEAR         = 2000
GLOBALSCALE  = 1.0
HEIGHT       = 0., 50., 100.
INPUTPATH    = '/data/emission/edgar/v4/2000'
CLASS(1)     = 'b10_2000_n2o.1x1', 1, 1.0
CLASS(2)     = 'b20_2000_n2o.1x1', 1, 0.8
CLASS(3)     = 'b20_2000_n2o.1x1', 2, 0.1
CLASS(4)     = 'b20_2000_n2o.1x1', 3, 0.1
CLASS(5)     = 'b30_2000_n2o.1x1', 2, 3.0
CLASS(6)     = 'b40_2000_n2o.1x1', 1, 1.0
/
```

Figure 2: Example for an EDGAR2NC namelist

level index) is, however, not possible, since the parameter dimension is then already used for the number of variables. For more detailed information see the NCREGRID documentations Jöckel (2006) and `http://www.mpch-mainz.mpg.de/~joeckel/ncregrid/`.

With these rules, the emission *type* is automatically detected by OFFLEM from the NCREGRID import method (`FILE` or `VAR`), the number of imported variables (N_{var}), the number of imported data levels (N_{lev}), the number of imported invariant parameters (N_{par}), and the presence of emission heights. Table 1 lists all possible combinations of dimensions and specifiers resulting in a specific emission *type*. All other combinations are inconsistent and will terminate the simulation.

3   Creating OFFLEM input files with EDGAR2NC

In order to further facilitate the creation of emission data files for OFFLEM, specifically 2D and Nx2D fluxes, the preprocessing tool EDGAR2NC is provided. EDGAR2NC automatically detects the time resolution from the header of the ASCII-based EDGAR file format, which must contain the correct keyword, either "annual", "seasonal", or "monthly", resulting in a netCDF time axis of 1, 4, or 12 steps, respectively. In the namelist, the user can specify:

- `OUTPUT`: The name of the output file.

- `SPECIES`: The species (=variable) name.

- `L_MASSFLUX`: A switch for optional output of the data in original units (in general as mass-flux in $kg/(m^2s)$).

- `MOLARMASS`: The molar mass of the species for conversion to (molecules $m^{-2}s^{-1}$) as required by OFFLEM.
  A note of caution: The molar mass must be consistent with the mass units in the original file. For example the emissions for propane can be given in $kg(C_3H_8)/(m^2s)$ or into $kg(C)/(m^2s)$.)

- `YEAR`: The year of the emissions.

- `GLOBALSCALE`: A global scaling factor (e.g., to generate files for sensitivity studies w.r.t. global emission budgets or for converting the mass flux units, e.g. $kg(C)/(m^2s)$ in $kg(C_3H_8)/(m^2s)$).

- `HEIGHT`: A list (up to 100 levels) of geometric emission heights (in m).

- `INPUTPATH`: The input path of the ASCII-files.

- `CLASS(n)`: A list of emission classes. Up to 10000 classes are possible. An emission class consists of

  - The name of the ASCII-file.
  - The number of the level (level index corresponding to the emission height as specified above).
  - The fraction (or scaling factor) to be put at the respective level.

Note that the year and the list of emission heights are only included to keep the netCDF file fully self-describing: The keyword `Z=` in the OFFLEM namelist *action string* controls the distribution onto the levels for the model simulation.

An example namelist file is shown in Fig. 2. Here an N_2O emission file for the year 2000 named `'example.nc'` is created. N_2O has a molar mass of 44.02 g mol^{-1}. The new emission file distinguishes 3 emission heights (0, 50 and 100 meter). Thus a Nx2D emission file is built. As `L_MASSFLUX` is set .FALSE., only the emission flux in molecules m^{-2} s^{-1} will be calculated. No global scaling factor is applied (`GLOBALSCALE` =1.0). The original data files can be found in the directory `'/data/emission/edgar/v4/2000'`. The data of four files (`'b10_2000_n2o.1x1'`, `'b20_2000_n2o.1x1'`, `'b30_2000_n2o.1x1'` and `'b40_2000_n2o.1x1'`) are distributed into 3 emission layers. The emissions of the files `'b10_2000_n2o.1x1'` and `'b40_2000_n2o.1x1'` are completely assigned to the first emission height without any scaling factors (`class(1)` and `class(6)`). For emission `class(5)` three times the emissions contained in file `'b30_2000_n2o.1x1'` are put into the second emission layer (50 m height). The emissions of the file `'b20_2000_n2o.1x1'` are distributed over all three emission heights (`class(2)`, `class(3)` and `class(4)`). As the sum of the scaling factors of these classes is 1, the amount of the emission is the same as in the original file. 80%

import method	Z keyword	N_{var}	N_{lev}	N_{par}	emission *type*
OFFLEM	OFFLEM	NCREGRID	NCREGRID	NCREGRID	
VAR	NO	1	1	1	→ 2D
VAR	NO	1	nlev	1	→ 3D
FILE	NO	1,nvar	1	1,nvar	→ 2D
FILE	NO	1,nvar	nlev	1,nvar	→ 3D
VAR	YES	1	1	1,N	→ Nx2D

Table 1: The emission *type* for the OFFLEM algorithm is automatically detected by using information from the OFFLEM namelist file (offlem.nml) and the results from the data import interface (NCREGRID). The import method is VAR for one variable, or FILE for multiple variables from one file. Z indicates the presence of the Z= specifier in the OFFLEM namelist. N_{var} is the resulting number of imported variables, N_{lev} the number of imported data levels, and N_{par} the length of the imported invariant parameter dimension. The number of model layers is nlev, N the number of emission levels specified with Z=, and nvar>1 the number of imported variables. Combinations which are not shown are inconsistent and will terminate the simulation.

```
&CPL
tropopause = 'tropop','tp_i'
!            t1,  t2,   d1,    d2,               dtn, lat1,lat2, lev1,lev2, lon1,lon2, s
TNUDGE(8)  = 'CH4','',  'offlem','n002_CH4', 10800.0, -90.0,90.0,    0, 0, 0.0,360.0, T
TNUDGE(17) = 'O3s','',  'tracer_gp','O3',       -1.0, -90.0,90.0,   -2,-1, 0.0,360.0, T
```

Figure 3: Example for a TNUDGE namelist file: The tracer CH4 (methane) is nudged to a field named n002_CH4 provided by OFFLEM with a nudging coefficient of 10800 s^{-1}. The nudging is applied at the surface (0,0) of the entire globe (i.e., in the latitude range -90.0° to 90.0° and the longitude range 0.0° to 360.0°. The calculation of the corresponding flux is requested (s=T). The tracer 'O3s' is nudged to the ozone tracer O3. In this case hard-nudging is chosen (-1 as relaxation coefficient *dtn*) in the global stratosphere (i.e., *lev1*=-2) and the top of the atmosphere (*lev2*=-1)).

of the emissions are assigned to the lowest emission layer, whereas 10% of the emissions are assigned to the second and third layer, respectively.

4   Pseudo Emissions (TNUDGE)

The TNUDGE namelist file only consists of the coupling namelist &CPL. In order to provide the dynamical tropopause as a specific boundary for tracer nudging, TNUDGE is coupled to a submodel making this information available. The first entry tropopause accomplishes the import of the tropopause height index via the MESSy data transfer/export interface. In this case 'tropop' and 'tp_i' point to the submodel TROPOP, which provides the tropopause index named 'tp_i'.

The user specifies a pseudo-emission in the TNUDGE namelist file with 12 entries:

```
TNUDGE(n) = t1, t2, d1, d2, dtn,
            lat1, lat2,
            lev1, lev2,
            lon1, lon2, s
```

by defining

- The name of the tracer to be nudged. Note that tracers in MESSy are unambiguously identified by a name (*t1*) and a subname (*t2*).

- The name of the data field (in the MESSy data transfer/export interface) containing the prescribed mixing ratio to which the tracer is relaxed (two strings *d1* and *d2*). *d1* points to the submodel (e.g. OFFLEM) which provides the data field *d2*.

- The nudging coefficient (*dtn*, in seconds). If this coefficient is negative, hard nudging is applied, i.e. *dtn* is set to the model time step.

- The latitude range (*lat1, lat2*) where nudging is applied.

- The level index range (*lev1, lev2*) where nudging is applied. The order of *lev1* and *lev2* can be chosen arbitrarily. Positive integers are used for model layer index. Special levels for *lev1* and/or *lev2* are -2 (tropopause), -1 (top of the atmosphere), 0 (surface).

- The longitude range (*lon1, lon2*) where nudging is applied.

- A switch s, which is T (true) for calculating the corresponding diagnosed flux, and F (false), to omit this calculation.

As in OFFLEM, n is an arbitrary but unambiguous number in a list of namelist entries of the same type.

In TNUDGE, both 2-dimensional (e.g., only at the surface layer, *lev1, lev2* = 0,0) and 3-dimensional (e.g., the stratosphere, *lev1, lev2* = -2,-1) prescribed fields can be used for tracer nudging. Furthermore, a 2D field can also be nudged into a range of levels.

5   Calculated Emissions (ONLEM)

The ONLEM namelist file consists of two parts.

The first part (&RGTEVENTS) containing the RG_TRIG triggers is organized in a similar way as in the OFFLEM namelist file. Specific emissions are defined by one (or a list of) regridding triggers. The presence of the triggers determines if an emission is calculated or not. If an online emission does not require any input fields the keyword NO_RGT is given in the stepper action string of the respective RG_TRIG trigger. The number of regridding triggers per emission is determined by the number of required input fields for the calculation of the respective fluxes. The RG_TRIG triggers and thus the input files are assigned to a specific emission by the TYPE keyword. If more than one input field is needed for the calculation of an online emission, all triggers contain the same emission TYPE specifier. To perform the calculation of an online emission requiring more than one input field all RG_TRIG triggers belonging to this emission TYPE must be active, otherwise the simulation will terminate.

To summarize, the ONLEM stepper action string can contain the following keywords, separated by semicolons:

- TYPE= followed by a string defining a specific emission. All regridding triggers for one emission need to have the same TYPE. The TYPE is also used to choose a specific algorithm, in case alternatives are available (e.g., TYPE=SS_lsce or TYPE=SS_monahan) for the two alternative sea salt emission calculations).

- NO_RGT This keyword (without value!) is used if the online emission does not depend on external data (as for instance the sea salt emissions), but only on model parameters.

- NML= This keyword has the same functionality as in OFFLEM for the import of additional external data.

- FILE= This keyword has the same functionality as in OFFLEM for the import of additional external data.

The most important difference between the ONLEM and the OFFLEM algorithm is the way in which calculated fluxes are assigned to the corresponding tracers. In ONLEM, one emission algorithm can deliver multiple fluxes. Also, it might be desirable to attribute one specific flux to more than one tracer. The flux-to-tracer (F2T) association is placed in the coupling namelist (&CPL, the second part of the ONELM namelist) and is of the form

F2T(n) = *name, a1, a2, ...*

where *name* is the name of the field in the MESSy data transfer/export interface which contains the calculated ONLEM flux. (In this case it is sufficient to identify a field only by its object name and not as usually with two strings, because all these fluxes are calculated by ONLEM itself and thus the first string indicating the submodel providing the data is obsolete.). The *name*s of the fluxes of the individual emission types are defined hard-coded within the ONLEM submodel). *a1, a2, ...* are the association strings for all available tracer sets (currently, only one string (*a1*) is supported for the tracers in grid point space). The association string contains a semicolon-separated list of substrings, each starting with the name of the tracer, followed by a colon, followed by the comma separated keywords

- M= for the emission *method*, i.e., 0 (default), 1, or 2.

- SC= defining the fraction (or scaling factor) of the flux into the tracer (1.0 by default).

Several examples for online-calculated emissions are shown in Fig. 4. The namelist &RGTEVENTS lists regridding triggers for five different emission TYPEs. The syntax of the regridding trigger is described in detail in Section 2.

- RG_TRIG(1) triggers DMS emissions over the ocean (TYPE=DMS). The input file contains monthly mean DMS sea water concentrations. The name of the *counter* is set to DMS_sea.

- RG_TRIG(2) is the trigger for the sea salt emissions following Schulz. As these emissions do not depend on input data the *event* part of the namelist is empty and the *counter* is filled with dummy values. Only the *action string* is meaningful, containing the TYPE of the emission and the keyword NO_RGT indicating that the emission is independent of any input data.

- The same syntax applies for the sea salt emissions after Monahan. With the exclamation mark in front of RG_TRIG(3) this line is only a comment and therefore deactivated.

- RG_TRIG(14) triggers volatile organic compound (VOC) emissions (TYPE=VOC).

- The last emission TYPE (NO) needs four input files simultaneaously. These files contain monthly mean NO emission classes (RG_TRIG(17) and RG_TRIG(18)), the leaf area index (RG_TRIG(19))

```
&CPL
F2T(1) = 'emis_dms_sea', 'DMS:M=2,SC=1.0;',    ! DMS
F2T(4) = 'ISOP_emflux',  'ISOP:M=2,SC=0.6;',  ! VOC
F2T(5) = 'MTERP_emflux', 'MTERP:M=2,SC=1.0;', ! VOC
! example for multiple tracers:
F2T(6) = 'NO_emflux',    'NO:M=2,SC=0.6;NO2:M=2,SC=0.4;',    ! NO
/
&RGTEVENTS
! DMS emissions over water:
RG_TRIG(1)  = 1,'months','first',0, 'DMS_sea', 1,1,12,1, 'TYPE=DMS;
                                                NML=./onlem/seawater_DMS.nml'

! sea salt emissions:
! after M. Schulz:
RG_TRIG(2) = , , , ,               ,                 1,1,1,1,  'TYPE=SS_lsce; NO_RGT'
! after Monahan:
!RG_TRIG(3) = , , , ,              ,                 1,1,1,1,  'TYPE=SS_monahan; NO_RGT'
! VOC = isoprene, monoterpene:
RG_TRIG(14) = 1,'months','first',0, 'emis_VOC',   1,1,12,1, 'TYPE=VOC; NML=./onlem/emis_VOC.nml'
! NOx:
RG_TRIG(16) = 1,'months','first',0, 'emis_NO',    1,1,12,1, 'NML=./onlem/emis_NO.nml; TYPE=NO;'
RG_TRIG(17) = 1,'months','first',0, 'noemclass1', 1,1,12,1, 'TYPE=NO; VAR=noemclass1;
                                                NML=./onlem/NOemisclass1.nml'
RG_TRIG(18) = 1,'months','first',0, 'noemclass2', 1,1,12,1, 'TYPE=NO; VAR=noemclass2;
                                                NML=./onlem/NOemisclass2.nml'
RG_TRIG(19) = 1,'months','first',0, 'lai',        1,1,12,1, 'TYPE=NO;VAR=lai;
                                                NML=./onlem/surf_para_4l.nml'
/
```

Figure 4: Example for an ONLEM namelist file. The detailed description is given in the text

and data of the usage of fertilizers (`RG_TRIG(16)`). Remember that for each emission the whole block of the same emission `TYPE` must be commented in or out as all fields for this emission `TYPE` are needed for the calculation. Activating only a part of the `RG_TRIG` entries of one emission `TYPE` causes the simulation to terminate.

Apart from the keyword `NO_RGT` and the `TYPE` label, which are needed to organize the different emissions, all other entries and their meaning are the same as in the OFFLEM namelist file. The requested emissions are identified via the given `TYPE` argument. Thus the user can choose between the two different sea salt emissions (`RG_TRIG(2)` and `RG_TRIG(3)` in Fig. 4) `TYPE=SS_monahan` and `TYPE=SS_lsce`. The sea salt emissions are also a good example for emissions which do not require an external input field. Thus for both sea salt emissions the string contains the keyword `NO_RGT`.

The emission fluxes calculated by activating the `RG_TRIG` event can be directly assigned to gas phase tracers within ONLEM. This is done in the `&CPL` namelist. Each `F2T` entry connects one emission flux to one or more tracers:

- The DMS emission flux `emis_dms_sea` (which was

triggered by `RG_TRIG(1)`) is assigned by `F2T(1)` to the gas phase tracer DMS. The chosen *method* is 2, i.e. a lower boundary condition for the vertical diffusive flux of the DMS tracer is calculated from the emission flux.

- As the sea salt emission is an aerosol emission which can not be directly assigned to tracers, no F2T entry for the sea salt emission is given here.

- The emission `TYPE=VOC` results in two emission fluxes `ISOP_emflux` and `MTERP_emflux`, an isoprene and and monoterpene emission flux, which are assigned by `F2T(4)` and `F2T(5)`, respectively. In the example, the isoprene emission flux is scaled to 60% of the calculated flux.

- The NO emission flux is split: 60% of the flux goes into NO and 40% into NO_2.

For all these examples the emission method 2, i.e. a lower boundary condition for the diffusive flux was chosen. If no `F2T` entry is given for a gas phase emission the result is the same as if $method = 0$ is chosen.

6 Adding new emissions to ONLEM

As all emissions calculated in ONLEM are in some way dependent on the physical state of the atmosphere, adding a new emission to ONLEM requires the implementation of a new subroutine (which contains the parameterization of the emission) and some additional parameters. The new subroutine can simply be added to the ONLEM core file (`messy_onlem.f90`) and must be declared `PUBLIC` within the header of the module. For the implementation in the submodel interface layer of ONLEM (`messy_onlem_e5.f90`), five new entries are needed. Their locations are highlighted by the marker:

```
!#############################
! ### add new emission here ###
!#############################
```

In the order of the appearance of the markers in the code the following entries are required:

- In the header of the module:

  - Increase the number of emission `TYPE`s `max_emis` by 1 and add the new emission `TYPE` name to `emis_type`
  - Declare the pointer for the input fields (import triggered by `RG_TRIG`, one pointer per variable) and the output fields (the resulting emission fluxes).

- In `messy_onlem_init_memory`:
  Define the names and allocate the memory space for the input and output fields in the MESSy data transfer/export interface.

- In `messy_onlem_global_start`:
  Add item in `case` construct assigning the imported data (by NCREGRID) to the respective pointer.

- In `messy_onlem_vdiff`:
  Add item in `case` construct to call the new subroutine calculating the new emission flux.

Last but not least the respective entries in the namelist files must be set. First, as many `RG_TRIG` events must be added to `&RGTEVENTS` as input files are needed for the new emission. Second, the individual namelist files for NCREGRID requested by triggers must be made available. Finally, if the new subroutine provides a gas phase emission which should be directly assigned to a tracer, a `F2T` entry in the `&CPL` namelist must be given.

This is all that is required for the implementation of a new calculated emission. Everything else is automatic in ONLEM.

References

Jöckel, P.: Technical Note: Recursive rediscretisation of geo-scientific data in multiple dimensions in the Modular Earth Submodel System (MESSy) data import interface, Atmos. Chem. Phys. Disc., submitted, 2006.

Jöckel, P., Sander, R., Kerkweg, A., Tost, H., and Lelieveld, J.: Technical Note: The Modular Earth Submodel System (MESSy) - a new approach towards Earth System Modeling, Atmos. Chem. Phys., 5, 433–444, 2005.