Supplement of:
Methane chemistry in a nutshell – The new submodels CH4 (v1.0) and TRSYNC (v1.0) in MESSy (v2.54.0)

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1 Documentation of the CH4 submodel

1.1 Introduction

The CH4 submodel represents a simplified methane (CH_4) chemistry. It defines the tracer `CH4_fx`, which gets reduced via the four CH_4 sink reactions. The tracer is initialized from external data via TRACER (Jöckel et al., 2008) and modified by either emissions, which need to be introduced via the submodel OFFline EMISsions (OFFEMIS) (Kerkweg et al., 2006) or by Newtonian relaxation towards a lower boundary condition with the submodel TNUDGE (Kerkweg et al., 2006). Example namelist entries concerning the configuration of these submodels are found in Section 3.

Additional to that, the CH4 submodel provides two further options. One is the simulation of the CH_4 isotopologues, and the second is the representation of age- and emission classes of CH_4, which, to some extent, are able to resolve an additional spatial and temporal information of the CH_4 emissions.

The option concerning the CH_4 isotopologues can be applied with respect to carbon-13 (^{13}C) isotopologues, deuterium (D) isotopologues, or both. The submodel defines the following tracers for the given isotopologues: `CH4_12C` (methane containing carbon-12 (^{12}C, $^{12}CH_4$)), `CH4_13C` (methane containing ^{13}C ($^{13}CH_4$)), `CH4_D0` (CH_4), and `CH4_D1` (deuterated methane (CH_3D)).

The option to simulate age- and emission classes introduces additional tracers depending on the chosen number of age- and emission classes. For every combination of age- and emission class one tracer is defined, thus, if N is the number of age classes and M is the number of emission classes, in total $N \times M$ additional tracers are defined. The tracers are denoted by the names `CH4_fx_e[mm]_a[nn]`, with `[mm]` being the identifying number of the emission class and `[nn]` the number of the age class.

The following section documents the subroutines, which are part of the CH4 submodel and in the section "User interface" the entries in the corresponding namelists are explained.

1.2 MODULE messy_ch4_si: Subroutines in the submodel interface layer (SMIL)

These subroutines follow the general structure mandatory for Modular Earth Submodel System (MESSy) submodels. Note that _gp and _lg denote the Gaussian grid point and Lagrangian mode (see Brinkop and Jöckel (2019) for more information). In the presented examples solely the Gaussian grid point mode is used.

- `SUBROUTINE ch4_initialize`: Initializes the submodel, reads the control and coupling namelists and broadcasts the information to all parallel tasks.

- `SUBROUTINE ch4_new_tracer`: Defines the new tracers, which also includes the additional tracers regarding the submodel extensions (if applied).

- `SUBROUTINE ch4_init_memory`: Defines the channel objects and allocates memory.

- `SUBROUTINE ch4_init_coupling`: Sets pointers for coupling to the basemodel and other submodels.

– SUBROUTINE `ch4_global_start`: Sets values of internal variables with respect to the applied ageing method, if the option of age- and emission classes is switched on.

– SUBROUTINE `ch4_vdiff`: Currently not used.

– SUBROUTINE `ch4_physc`: This subroutine calls the integration step of the submodel, i.e. `ch4_integrate`. It further accounts for the water vapour (H_2O) feedback, if it is switched on. The tendencies for the age- and emission class tracers and the isotopologue tracers are calculated in separate integration routines, namely `class_integrate_gp/lg` and `iso_integrate_gp/lg`.

– SUBROUTINE `ch4_global_end`: Entry point in time loop for LG calculations; not used for the presented examples.

– SUBROUTINE `ch4_free_memory`: Deallocation of allocated memory.

1.3 MODULE messy_ch4: Subroutines in the submodel core layer (SMCL)

The following subroutines represent the core layer of the submodel.

SUBROUTINE ch4_integrate		(CH4_te, CH4, OH, O1D, Cl, j_CH4, temp, press, spechum, iso_id)	
name	type	intent	description
mandatory arguments:			
CH4_te	REAL	OUT	CH_4 tendency
CH4	REAL	IN	CH_4 mixing ratio
OH	REAL	IN	the hydroxyl radical (OH) mixing ratio
O1D	REAL	IN	excited oxygen ($O(^1D)$) mixing ratio
Cl	REAL	IN	chlorine (Cl) mixing ratio
j_CH4	REAL	IN	photolysis rate of CH_4
temp	REAL	IN	temperature
press	REAL	IN	pressure
spechum	REAL	IN	specific humidity
iso_id	INTEGER	IN	ID of isotopologue

description:

This subroutine executes the integration step of the submodel. It applies the functional (i.e. temperature dependent) reaction rate coefficients of the sink reactions of CH_4 and accounts for the Kinetic Isotope Effect (KIE) in the case of rare isotopologues.

SUBROUTINE sca_tend		(m, mte, s, ste, dt, a)	
name	type	intent	description
mandatory arguments:			
m	REAL	IN	master tracer
mte	REAL	IN	tendency of master tracer
s	REAL	IN	sum of fractional tracers
ste	REAL	IN	sum of fractional tracer tendencies
dt	REAL	IN	time step length
a	REAL	OUT	resulting correction factor
description:			
Calculates the necessary correction factor so that the fractional tracers including their tendencies add up to the master tracer (incl. its current tendency).			

SUBROUTINE adj_tend		(f, t, a, dt, tadj)	
name	type	intent	description
mandatory arguments:			
f	REAL	IN	fractional tracer
t	REAL	IN	tendency of fractional tracer
a	REAL	IN	correction factor
dt	REAL	IN	time step length
tadj	REAL	OUT	resulting additional tendency for adjustment
description:			
Calculates the necessary additional tendency to adjust for the given correction factor.			

SUBROUTINE ch4_read_nml_ctrl		(status, iou)	
name	type	intent	description
mandatory arguments:			
status	INTEGER	OUT	error status info
iou	INTEGER	IN	I/O unit
description:			
This subroutine is used to read the CTRL-namelist of the submodel.			

1.4 Private subroutines

Private subroutines in `messy_ch4_si`

SUBROUTINE ch4_read_nml_cpl		(status, iou)	
name	type	intent	description
mandatory arguments:			
status	INTEGER	OUT	error status info
iou	INTEGER	IN	I/O unit
description:			
This subroutine is used to read the CPL-namelist of the submodel.			

SUBROUTINE class_integrate_gp		(temp, press, spechum)	
name	type	intent	description
mandatory arguments:			
temp	REAL, DIMENSION(:,:)	IN	temperature
press	REAL, DIMENSION(:,:)	IN	pressure
spechum	REAL, DIMENSION(:,:)	IN	specific humidity
description:			
This subroutine calls `ch4_integrate` for every age- and emission class tracer separately.			

SUBROUTINE class_age_move_gp		(CH4c, CH4c_te)	
name	type	intent	description
mandatory arguments:			
CH4c	REAL, DIMENSION(:,:)	IN	current CH_4 tracer mixing ratio
CH4c_te	REAL, DIMENSION(:,:)	IN	current CH_4 tracer tendency
description:			
Accounts for the shifting from one age class to the next.			

SUBROUTINE class_adj_tend_gp		(CH4c, CH4c_te)	
name	type	intent	description
mandatory arguments:			
CH4c	REAL, DIMENSION(:,:)	IN	current CH_4 tracer mixing ratio
CH4c_te	REAL, DIMENSION(:,:)	IN	current CH_4 tracer tendency
description:			
Adjusts the tendencies of the age- and emission class tracers so that the tracers sum up to the master tracer CH4_fx, which is required to correct for potential numerical inaccuracies.			

SUBROUTINE iso_integrate_gp		(temp, press, spechum, CH4_te)	
name	type	intent	description
mandatory arguments:			
temp	REAL, DIMENSION(:,:)	IN	temperature
press	REAL, DIMENSION(:,:)	IN	pressure
spechum	REAL, DIMENSION(:,:)	IN	specific humidity
CH4_te	REAL, DIMENSION(:,:)	IN	current CH_4 tracer tendency

description:

Calls `ch4_integrate` for every isotopologue tracer separately. It further calculates the tendency added to the deuterated water vapour (HDO), either by the simple assumption that one HDO molecule is produced by one oxidized CH_3D molecule, or by the function

$$\frac{\partial(HDO)}{\partial t} = \frac{-\frac{\partial(CH_3D)}{\partial t} + 6.32 \times 10^{-5} \cdot \frac{\partial(CH_4)}{\partial t}}{\frac{M_{air}}{M_{HDO}}\left(\frac{1}{1-HDO}\right)^2}, \quad (1)$$

proposed by Eichinger et al. (2015).

SUBROUTINE class_adj_tend_gp		(CH4c, CH4c_te, idt_gp_iso_adj)	
name	type	intent	description
mandatory arguments:			
CH4c	REAL, DIMENSION(:)	IN	current CH_4 tracer mixing ratio
CH4c_te	REAL, DIMENSION(:)	IN	current CH_4 tracer tendency
idt_gp_iso_adj	REAL, DIMENSION(:)	IN	list of tracer IDs

description:

Adjusts the tendencies of the isotopologue tracers so that the tracers regarding the isotopes of the same element sum up to the master tracer `CH4_fx`, which is required to correct for potential numerical inaccuracies.

Private subroutines in `messy_ch4`

SUBROUTINE calc_KIE		(KIE_AB_val, temp_t, KIE_t)	
name	type	intent	description
mandatory arguments:			
KIE_AB_val	REAL, DIMENSION(2)	IN	KIE parameters A and B
temp_t	REAL	IN	temperature
KIE_t	REAL	OUT	KIE value
description:			
Calculates the KIE with the equation: KIE_t = A·exp(B/temp).			

1.5 User interface

1.5.1 CH4 CTRL namelist

The control (CTRL) namelist of the CH4 submodel includes the KIE values applied in the isotopologue extension of the submodel for all four sink reactions and both isotopologues.

The KIE is represented in the form KIE $=$ A$\cdot\exp(\mathrm{B}/T)$, with A and B being the individual parameters and T the temperature in [K]. The namelist entries are given therefore as:

KIE_CH4_XX_YY = A, B.

XX and YY are set according to the specified reaction. XX denotes thereby the isotope in CH_4 and is 13C or D1. YY defines the reaction partner (either OH, O1D or CL) as well as the photolysis with jval. For those KIE, which are temperature independent, B is set to 0.0. The default values are A = 1.0 and B = 0.0, so that no KIE is applied.

1.5.2 CH4 CPL namelist

The coupling (CPL) namelist of the CH4 submodel sets the parameters for the applied extensions and feedback on the specific humidity. It further determines the channel objects used as the reaction partners in the CH_4 oxidation.

- i_H2O_feedback takes an integer, which controls the feedback of CH_4 oxidation on the specific humidity. Allowed values are: 0: no feedback, 1: feedback from GP and 2: feedback from LG. GP and LG denote grid-point representation and Lagrangian representation, respectively. (Default: 0)

- l_ef_re is a logical switch indicating whether the empirical formula introduced by Eichinger et al. (2015) is used (T) or not (F). (Default: F)

- L_GP and L_LG are both logical switches implying whether the Gaussian representation (GP) or Lagrangian representation (LG), or both are applied. The following namelist entries are shown for GP, however, there a identical entries for LG as well (indicated by gp and lg, respectively). (Default: L_GP = T, L_LG = F)
- c_gp_OH, c_gp_O1D, c_gp_Cl and c_gp_jCH4 define the chosen channel objects for the reaction partners of CH_4. They take two strings, the first indicates the channel, the second the object name.
- i_gp_nclass_emis_age denotes the number of emission- and age classes. It takes two integers, the first is the number of emission classes, the second is the number of age classes. (Default: i_gp_nclass_emis_age = 0, 0,)
- r_gp_age_cll is an optional entry, which adjusts the time period (in days) of one age class. This entry is only valid for ageing option 1 and 2 (see main text section 3.1). (Default: 30.44 for each age class)
- l_gp_adj_tend is a logical switch, which indicates whether the tendencies are adjusted so that the additional age- and emission class tracers sum up to the master tracer CH4_fx. (Default: T)
- i_gp_ageing is an integer switch indicating the ageing method, which means the advancing of CH_4 from one age class to the next older one. It can be chosen between:
  - 0: monthly in one step
  - 1: continuously (default)
  - 2: monthly

  Note, using the first one, the Leapfrog time stepping with the Asselin-filter might cause numerical oscillations with negative values. Furthermore, the last one is not conform with the submodel TENDENCY, hence the corresponding diagnostic output created by TENDENCY is not meaningful. (Default: 1)
- l_gp_iso_C and l_gp_iso_H are logical switches. indicating whether the isotopologues of CH_4 concerning ^{13}C, D, or both are simulated. (Default: .FALSE.)

1.6 Example namelist

Namelist 1. Control (CTRL) and coupling (CPL) namelist of submodel CH4, stored in ch4.nml

```
&CTRL
!! ### KIE values for isotopologues
!! ### SYNTAX:
!! ###   KIE_*    = A, B,
!! ### with KIE(T) = A * exp(B/T)
!! ### temperature independent for B = 0._dp
!! ###
```

```
!! ### Reference KIE values:
!! ### Carbon 13 and D kinetic isotope effects in the reactions of CH4
!! ### with O1(D) and OH: New laboratory measurements and their
!! ### implications for the isotopic composition of stratospheric
!! ### methane
!! ### G. Saueressig, J. Crowley, P. Bergamaschi, C. Bruehl,
!! ### C.A.M. Brenninkmeijer and H. Fischer
!! ### [2001] Journal of Geosphysical Research
KIE_CH4_13C_OH  = 1.0039, 0.0,
KIE_CH4_13C_O1D = 1.013 , 0.0,
KIE_CH4_13C_CL  = 1.043 , 6.455,
KIE_CH4_13C_jval = 1.0 , 0.0,
KIE_CH4_D1_OH   = 1.097 , 49.0,
KIE_CH4_D1_O1D  = 1.060 , 0.0,
KIE_CH4_D1_CL   = 1.278 , 51.31,
KIE_CH4_D1_jval = 1.0, 0.0,
!
/
!
&CPL
!! ### feed back H2O tendency (= -2 * CH4-tendency) into specfic humidity?
!! ### (0: no feedback; 1: feedback from GP; 2: feedback from LG)
i_H2O_feedback = 1,
!! ### grid-point calculation
L_GP = T,
! L_LG = T,
!! ### educts and photolysis rate
c_gp_OH   = 'import_grid', 'CH4OX_OH',
c_gp_O1D  = 'import_grid', 'CH4OX_O1D',
c_gp_Cl   = 'import_grid', 'CH4OX_Cl',
c_gp_jCH4 = 'jval_gp',     'J_CH4',
!
! flag for empirical formula of Eichinger et al. (2015)
l_ef_re = T,
!
! #####################################################
! ### ADDITIONAL SECTION FOR EMISSION AND AGE CLASSES ###
! #####################################################
!
! ### n emission x m age classes
i_gp_nclass_emis_age = 48, 4, ! CAREFUL: If age / emis classes are changed
                              ! here, the tracer.nml must be updated
                              ! apropriately!
                              ! For emissions check offemis.nml,too
```

```
! ### age class duration [days] (only for ageing method 1)
!r_gp_age_cll = 1.0, 1.0, 1.0, 1.0,          ! for testing
!r_gp_age_cll = 30.44, 30.44, 30.44,30.44,  ! default
! ### adjust tendencies to sum tracer (default: true)
!l_gp_adj_tend = T,
! ### ageing method (0: monthly in one step, 1: continuous (default),
! ###                2: monthly, not TENDENCY conform)
!i_gp_ageing = 1,
i_gp_ageing = 2,
!
! ### n emission x m age classes
! i_lg_nclass_emis_age = 6, 4,
! ### age class duration [days] (only for ageing method 1)
!r_lg_age_cll = 1.0, 1.0, 1.0, 1.0,          ! for testing
!r_lg_age_cll = 30.44, 30.44, 30.44,30.44,   !
! ### adjust tendencies to sum tracer (default: true)
!l_lg_adj_tend = T,
! ### ageing method (0: monthly in one step, 1: continuous (default),
! ###                2: monthly, not TENDENCY conform)
!i_lg_ageing = 1,
! i_lg_ageing = 2,
!
! ############################################
! ### ADDITIONAL SECTION FOR ISOTOPOLOGUES ###
! ############################################
!
! ### Switch for isotopologues (GP)
l_gp_iso_C = .TRUE.
l_gp_iso_H = .TRUE.
! ### Switch for isotopologues (LG)
! l_lg_iso_C = .TRUE.
! l_lg_iso_H = .TRUE.
/
```

2 Documentation of the TRSYNC submodel

2.1 Introduction

The submodel TRacer SYNChronization (TRSYNC) guarantees that the physical H_2O tracers (incl. their isotopologues) receive also the correct tendencies of the corresponding chemical tracers.

The submodel for simplified CH_4 chemistry (CH4) defines the tracer `HDO`, the submodel H_2O ISOtopologues (H2OISO) defines `H2OISOHDOvap`, and the kinetic chemistry tagging technique (MECCA_TAG) in the Module Efficiently Calculating the Chemistry of the Atmosphere (MECCA) defines `I2H2O` (or a different idiom, chosen by the user). The auxiliary submodel TRSYNC couples these tracers to combine the physical and chemical isotopic fractionation.

Without any isotopological extension solely the 5th generation European Centre Hamburg general circulation model (ECHAM5) intrinsic tracer for specific humidity (q) is present. In this case, chemically produced H_2O (either from CH4 or from MECCA) directly adds optionally to q. However, in case of an isotopological extension using H2OISO, CH4 and/or MECCA_TAG the following additional tracers are defined:

- `H2OISOHHOvap` and `H2OISOHDOvap` (defined by H2OISO): The former is the total water tracer and the latter is the tracer of the rare isotopologue. Note that in H2OISO the two tracers do not add up to a master tracer, actually, `H2OISOHHOvap` represents and is identical to the master tracer (i.e. q).

- `HDO` (defined by CH4).

- `I1H2O` and `I2H2O`, representing H_2O and HDO, respectively (defined by MECCA_TAG): Both sum up to the chemical master tracer `H2O`.

- `H2O` (defined by MECCA): This tracer is originally not defined in MECCA, but is necessary in combination with MECCA_TAG for the internal scaling of `I1H2O` and `I2H2O`.

Figure S1 depicts the schematics of the coupling. At the beginning of every time step, `H2OISOHHOvap` is set to the current value of q, correcting any numerical deviations of `H2OISOHHOvap` from q caused in the previous time step. Next, basically all tracers are modified by the same physical processes: advection, vertical diffusion and convection. However, for the submodels E5VDIFF, CONVECT and CLOUD the hydrological processes are doubled in H2OISO to allow for isotope effects. The submodel Multi-phase Stratospheric Box Model (MSBM) calculates a tendency for q, which is added to `H2OISOHHOvap` as well. An equivalent tendency is added to `H2OISOHDOvap`, which is derived such that no additional fractionation by the multi-phase stratospheric chemistry is implied.

After all physical processes are complete, the submodel TRSYNC is called. It takes care that all tendencies of the previous (physical) processes of `HDO` and `I2H2O` are deleted and overwritten by the corresponding tendencies of the H2OISO equivalent `H2OISOHDOvap`. `I1H2O` is exceptional, as it must be set to the difference of the total tracer `H2OISOHHOvap` and the rare isotopologue `H2OISOHDOvap`. Note that for technical reasons the tracer `H2OISOHDOvap` is defined as one half of the corresponding chemical isotopological tracers `HDO` and `I2H2O`.

Next CH4 computes the CH_4 oxidation and derives the feedback onto q and HDO. At the very beginning of MECCA, the intrinsic `H2O` tracer is synchronized with q. Before and after the calls of the kinetic solver, `I1H2O` and `I2H2O` are scaled appropriately to add up to `H2O`. After this, the feedback onto H_2O is passed to q. To be precise, the sketch in Fig. S1 suggests that CH4 and MECCA are executed in the same simulation. This is indeed possible, but not necessary and it is important to note that only one of the two can provide the chemical feedback onto q, which can be arranged by corresponding switches in the namelists.

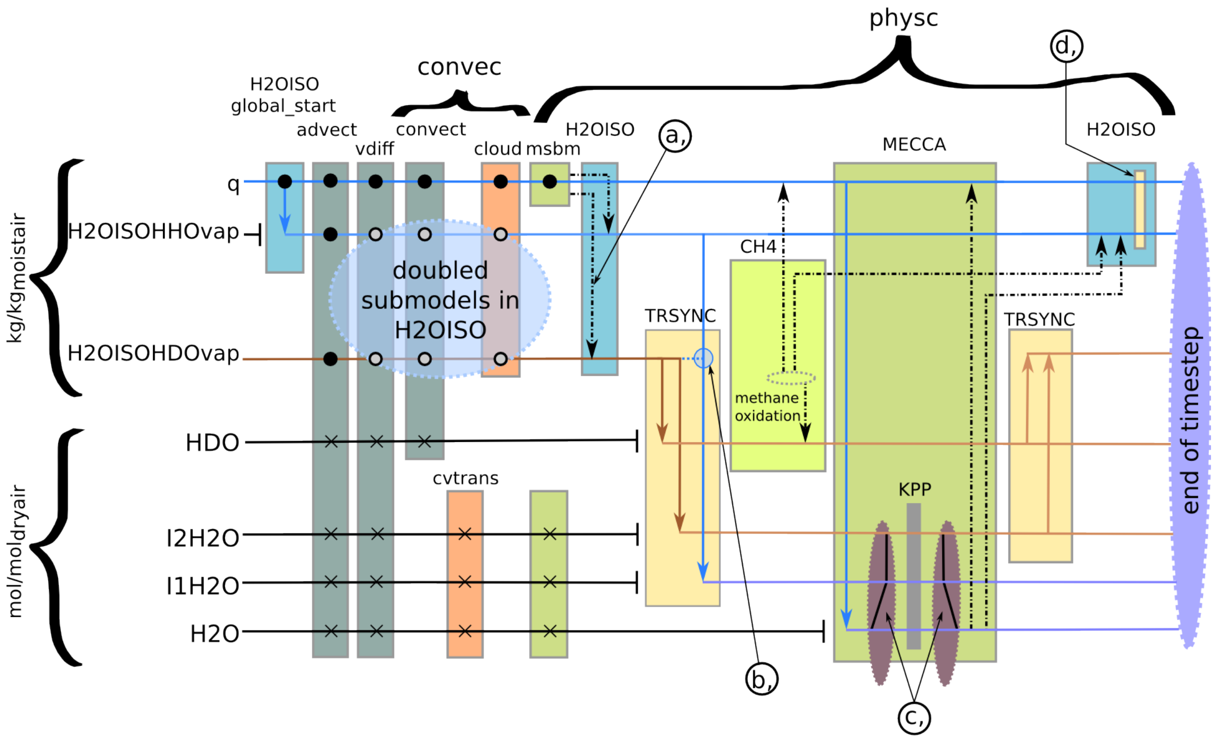

Figure S1. Sketch depicting the coupling of the hydrological cycle tracers in ECHAM/MESSy Atmospheric Chemistry (EMAC). q is the intrinsic variable of ECHAM5 for specific humidity. Similar, `H2OISOHHOvap` and `H2OISOHDOvap` are defined by H2OISO. q, `H2OISOHHOvap` and `H2OISOHDOvap` are in units kg of the tracer per kg of moist air (kg $\text{kg}^{-1}_{\text{moist air}}$). `HDO` is defined by CH4, `H2O` is defined by MECCA, and `I1H2O` and `I2H2O` are defined by MECCA-TAG in moles of the chemical tracer per mole of air (mol $\text{mol}^{-1})_{\text{dry air}}$. Arrows with dashed lines indicate that solely tendencies are added. Solid arrow lines correspond to a replacement of the contents. (a) relative tendency of MSBM of HHO tracer without fractionation, (b) sets `I1H2O` to the mol $\text{mol}^{-1}{}_{\text{dry air}}$ equivalent of `H2OISOHHOvap` - 2·`H2OISOHDOvap`, (c) adjusts `I1H2O` and `I2H2O` so that `I1H2O` + `I2H2O` = `H2O`, (d) numerical adjustment to ensure that the tendency of `H2OISOHHOvap` is equal to the tendency of q.

After the chemical processes, TRSYNC synchronizes the tracers `HDO` or `I2H2O` backward onto `H2OISOHDOvap`, and H2OISO also adds the chemical tendency of q to `H2OISOHHOvap`. As a last step H2OISO adjusts the tendency of `H2OISOHHOvap` so that it is conform to the tendency of q.

The following section documents the subroutines, which are part of the TRSYNC submodel and in the section “User interface” the entries of the corresponding namelist are explained.

2.2 MODULE messy_trsync_si: Subroutines in SMIL

These subroutines follow the general structure mandatory for MESSy submodels.

– `SUBROUTINE trsync_initialize`: Initializes the submodel, reads the coupling namelist and broadcasts necessary information to all parallel tasks.

– `SUBROUTINE trsync_init_memory`: Registers the tracers for the TENDENCY submodel, if the latter is applied.

– `SUBROUTINE trsync_init_coupling`: Sets pointers to the used tracers and checks whether the synchronized tracers are identical in terms of their molar mass.

– `SUBROUTINE trsync_init_tracer`: Initializes the tracers, hence checks whether the tracers are already initialized and accounts for a synchronized initial state.

– `SUBROUTINE trsync_physc`: This subroutine is called two times. The first time before the kinetic integrations of CH4 and MECCA and the second time after. It provides the necessary unit conversion and numerical adjustment to synchronize the chosen tracers.

– `SUBROUTINE trsync_free_memory`: Currently not necessary.

2.3 MODULE messy_trsync: Subroutines in SMCL

The following subroutines represent the core layer of the submodel.

SUBROUTINE convert_unit		(traten, case, type, molarmass, spechum, spechum_te, tracer)	
name	type	intent	description
mandatory arguments:			
traten	REAL	INOUT	tracer or tendency to be converted
case	INTEGER	IN	case of conversion (1: kg/kg⇒mol/mol or 2: mol/mol⇒kg/kg)
type	INTEGER	IN	type of conversion (1: tracer or 2: tendency)
molarmass	REAL	IN	molar mass of the converted tracer
spechum	REAL	IN	specific humidity
optional arguments:			
spechum_te	REAL	IN	tendency of specific humidity
tracer	REAL	IN	additional tracer mixing ratio if traten indicates the tendency
description:			
This subroutine calls the private subroutines convert_to_molmol, convert_to_kgkg, convert_to_molmol_te and convert_to_kgkg_te, depending on the chosen case and type.			

2.4 Private subroutines

Private subroutines in `messy_trsync_si`

SUBROUTINE trsync_read_nml_cpl		(status, iou)	
name	type	intent	description
mandatory arguments:			
`status`	`INTEGER`	OUT	error status info
`iou`	`INTEGER`	IN	I/O unit
description:			
This subroutine is used to read the CPL-namelist of the submodel.			

Private subroutines in `messy_trsync`

SUBROUTINE convert_to_kgkg		(tr_a, molarmass, spechum)	
name	type	intent	description
mandatory arguments:			
`tr_a`	`REAL`	INOUT	tracer in mol ${mol^{-1}}_{\text{dry air}}$ to be converted
`molarmass`	`REAL`	IN	molar mass of the converted tracer
`spechum`	`REAL`	IN	specific humidity
description:			
This subroutine converts the tracer `tr_a` from mol ${mol^{-1}}_{\text{dry air}}$ to kg $kg^{-1}_{\text{moist air}}$.			

SUBROUTINE convert_to_molmol		(tr_b, molarmass, spechum)	
name	type	intent	description
mandatory arguments:			
`tr_b`	`REAL`	INOUT	tracer in kg $kg^{-1}_{\text{moist air}}$ to be converted
`molarmass`	`REAL`	IN	molar mass of the converted tracer
`spechum`	`REAL`	IN	specific humidity
description:			
This subroutine converts the tracer `tr_b` from kg $kg^{-1}_{\text{moist air}}$ to mol ${mol^{-1}}_{\text{dry air}}$.			

SUBROUTINE convert_kgkg_te		(tr_a_te, tr_a, molarmass, spechum, spechum_te)	
name	type	intent	description
mandatory arguments:			
tr_a_te	REAL	INOUT	tendency in mol $\text{mol}^{-1}{}_{\text{dry air}}$ s^{-1} to be converted
tr_a	REAL	IN	corresponding tracer of tendency to be converted
molarmass	REAL	IN	molar mass of the converted tracer
spechum	REAL	IN	specific humidity
spechum_te	REAL	IN	tendency of specific humidity

description:

This subroutine converts the tendency `tr_a_te` from mol $\text{mol}^{-1}{}_{\text{dry air}}$ s^{-1} to kg $\text{kg}^{-1}_{\text{moist air}}$ s^{-1}.

SUBROUTINE convert_molmol_te		(tr_b_te, tr_b, molarmass, spechum, spechum_te)	
name	type	intent	description
mandatory arguments:			
tr_b_te	REAL	INOUT	tendency in kg $\text{kg}^{-1}_{\text{moist air}}$ s^{-1} to be converted
tr_b	REAL	IN	corresponding tracer of tendency to be converted
molarmass	REAL	IN	molar mass of the converted tracer
spechum	REAL	IN	specific humidity
spechum_te	REAL	IN	tendency of specific humidity

description:

This subroutine converts the tendency `tr_b_te` from kg $\text{kg}^{-1}_{\text{moist air}}$ s^{-1} to mol $\text{mol}^{-1}{}_{\text{dry air}}$ s^{-1}.

2.5 User interface

2.5.1 TRSYNC CPL namelist

The coupling (`CPL`) namelist of the TRSYNC submodel lists the tracers to be synchronized.

`TRSYNC` takes two strings and one integer switch. The first string indicates the chemical tracer in mol $mol^{-1}{}_{\text{dry air}}$. The second string indicates the physical tracer in kg $kg^{-1}_{\text{moist air}}$. The integer string denotes, whether the synchronization is done in both ways (`0`), the chemical tracer is synchronized by the physical tracer before chemistry only (`1`), or the physical tracer is synchronized by the chemical tracer after chemistry (`2`).

2.6 Example namelist

Namelist 2. Control (CTRL) and coupling (CPL) namelists of submodel TRSYNC stored in trsync.nml

```
&CTRL
/
!
&CPL
!! ### List of tracer which should be synchronized by TRSYNC
!! ###
!! ### TRSYNC : synchronization of HDO tracer
!! ### TRSYNC(1) = 'TR_A','TR_B',i
!! ### with:
!! ###       TR_A in mol/mol_dryair
!! ###       TR_B in kg/kg_moistair
!! ###
!! ### i = 0: both ways (default)
!! ###     1: chemical tracer is synchronized with physical tracer only
!! ###     2: physical tracer is synchronized with chemical tracer only
!! ###
!! ### trsync_physc(1) will synchronize TR_A with TR_B (=> TR_A will be overwritten)
!! ### trsync_physc(2) will synchronize TR_B with TR_A (=> TR_B will be overwritten)
!! ###
TRSYNC(1) = 'HDO', 'H2OISOHDOvap',
!! ### TRSYNC(1) = 'I2H2O', 'H2OISOHDOvap', 0,
!! ### Future:
!! ### TRSYNC(2) = '','H2OISOHH18Ovap', 0,
!! ### TRSYNC(3) = '','H2OISOHH17Ovap', 0,
/
```

3 Example namelist entries for other submodels corresponding to CH4 set-up

The following snippets show namelist entries of other submodels for a MESSy set-up with the CH4 submodel.

3.1 TRACER

Namelist 3. Part of tracer.nml to import initial values of CH_4 tracer.

```
! Import from first spin-up
&regrid
infile    = "~/EMAC-x-02_____0013_restart_0005_tracer_gp.nc",  ! 2010-12-31 23:48 ...
i_latm    = "lat",          ! name of latitude axis in input file
i_latr    = -90.0,90.0,     ! range of latitude axis in input file
i_lonm    = "lon",          ! name of longitude axis in input file
i_lonr    = 0.0,360.0,      ! range of longitude axis in input file
! No time coordinate in restart files
!i_timem   = "time",         ! name of time axis in input file
i_hyam    = "hyam",     ! name of hybrid A coefficients in input file
i_hybm    = "hybm",     ! name of hybrid B coefficients in input file
i_ps      = "101325.0 Pa",
i_p0      = "1. Pa",        ! value of reference pressure in input file
pressure  = F,
! Use ALL tracers in init file
!var       =  "CH4_fx;CH4_12C;CH4_13C;CH4_D0;CH4_D1", ! CH4 tracers
! No time coordinate in restart files
!i_t       = 25,
/
```

3.2 DDEP

Namelist 4. Configuration of ddep.nml to simulate soil-loss of CH_4.

```
!## SYNTAX:
!## import_predepvel(.) = 'channel', 'object', 'tracer-name', diag. flux calc.?
!## Note: channel object is deposition flux aand must be in [molec/m^2/s]
!
!
import_predepvel(1) = 'import_grid', 'DVMETH_oxid', 'CH4_fx', T,
import_predepvel(2) = 'import_grid', 'DVMETH_oxid', 'CH4_D0', T,
import_predepvel(3) = 'import_grid', 'DVMETH_CH3D_oxid', 'CH4_D1', T,
import_predepvel(4) = 'import_grid', 'DVMETH_13CH4_oxid', 'CH4_13C', T,
import_predepvel(5) = 'import_grid', 'DVMETH_oxid', 'CH4_12C', T,
!
```

3.3 IMPORT

Namelist 5. Entries of import.nml, which import the educts (OH, Cl and O(^{1}D)) from an earlier simulation and the CH_4 emission inventory for each emission class.

```
! ##########################################################################
! CH4
! ##########################################################################
!
! PRESCRIBED EDUCTS (CH + ...): OH, O1D, Cl for methane oxidation
! QCTM data starts at Dec 1978 and ends at Nov 2014
RG_TRIG(3)  = 1,’months’, ’first’,0, ’CH4OX’,  422,1,432,134,
        ’NML=./import/MISC/QCTM/ESCiMo_DLR1.0_RC1SD-base-10_4QCTM_misc_197901-201412.nml;’,
!
! ##########################################################################
! OFFEMIS
! ##########################################################################
!
! CH4_fx emissions
!
! biomass burning
RG_TRIG(20)  = 1,  ’months’, ’first’,0, ’BB_AUS’,        265,1,276,1,
        ’NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_bb+AUS_CH4_199001-201212.nml; VAR=CH4;’,
RG_TRIG(21)  = 1,  ’months’, ’first’,0, ’BB_CHINA’,      265,1,276,1,
        ’NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_bb+CHINA_CH4_199001-201212.nml; VAR=CH4;’,
RG_TRIG(22)  = 1,  ’months’, ’first’,0, ’BB_EU’,         265,1,276,1,
        ’NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_bb+EU_CH4_199001-201212.nml; VAR=CH4;’,
RG_TRIG(23)  = 1,  ’months’, ’first’,0, ’BB_INDIA’,      265,1,276,1,
        ’NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_bb+INDIA_CH4_199001-201212.nml; VAR=CH4;’,
RG_TRIG(24)  = 1,  ’months’, ’first’,0, ’BB_NA_bor’,     265,1,276,1,
        ’NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_bb+NAbor_CH4_199001-201212.nml; VAR=CH4;’,
RG_TRIG(25)  = 1,  ’months’, ’first’,0, ’BB_N_AFR’,      265,1,276,1,
        ’NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_bb+NAFR_CH4_199001-201212.nml; VAR=CH4;’,
RG_TRIG(26)  = 1,  ’months’, ’first’,0, ’BB_NA_temp’,    265,1,276,1,
        ’NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_bb+NAtemp_CH4_199001-201212.nml; VAR=CH4;’,
RG_TRIG(27)  = 1,  ’months’, ’first’,0, ’BB_N_MIDEAST’,  265,1,276,1,
        ’NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_bb+NMIDEAST_CH4_199001-201212.nml; VAR=CH4;’,
RG_TRIG(28)  = 1,  ’months’, ’first’,0, ’BB_RUS’,        265,1,276,1,
        ’NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_bb+RUS_CH4_199001-201212.nml; VAR=CH4;’,
RG_TRIG(29)  = 1,  ’months’, ’first’,0, ’BB_S_AFR’,      265,1,276,1,
        ’NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_bb+SAFR_CH4_199001-201212.nml; VAR=CH4;’,
RG_TRIG(30)  = 1,  ’months’, ’first’,0, ’BB_SA_temp’,    265,1,276,1,
        ’NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_bb+SAtemp_CH4_199001-201212.nml; VAR=CH4;’,
RG_TRIG(31)  = 1,  ’months’, ’first’,0, ’BB_SA_trop’,    265,1,276,1,
        ’NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_bb+SAtrop_CH4_199001-201212.nml; VAR=CH4;’,
```

```
RG_TRIG(32)  = 1,  'months', 'first',0, 'BB_SE_ASIA',    265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_bb+SEASIA_CH4_199001-201212.nml; VAR=CH4;',
!
! anthropogenic
!
RG_TRIG(140) = 1,  'months',  'first',0, 'Mfx_an_AFRICA',  265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_anth+AFRICA_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(141) = 1,  'months',  'first',0, 'Mfx_an_AUS',     265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_anth+AUS_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(142) = 1,  'months',  'first',0, 'Mfx_an_CHINA',   265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_anth+CHINA_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(143) = 1,  'months',  'first',0, 'Mfx_an_EU',      265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_anth+EU_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(144) = 1,  'months',  'first',0, 'Mfx_an_INDIA',   265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_anth+INDIA_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(145) = 1,  'months',  'first',0, 'Mfx_an_MIDEAST', 265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_anth+MIDEAST_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(146) = 1,  'months',  'first',0, 'Mfx_an_NA',      265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_anth+NA_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(147) = 1,  'months',  'first',0, 'Mfx_an_OCEAN',   265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_ship_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(148) = 1,  'months',  'first',0, 'Mfx_an_RUS',     265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_anth+RUS_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(149) = 1,  'months',  'first',0, 'Mfx_an_SA',      265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_anth+SA_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(150) = 1,  'months',  'first',0, 'Mfx_an_SE_ASIA', 265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_anth+SEASIA_CH4_199001-201212.nml; VAR=CH4;',
!
! ocean
!
RG_TRIG(151) = 1,  'months',  'first',0, 'Mfx_oc',         265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_ocean_CH4_199001-201212.nml; VAR=CH4;',
!
! rice
!
RG_TRIG(152) = 1,  'months', 'first',0, 'Mfx_ri_AFR',      265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_rice+AFR_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(153) = 1,  'months', 'first',0, 'Mfx_ri_ASIA_AUS', 265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_rice+ASIA+AUS_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(154) = 1,  'months', 'first',0, 'Mfx_ri_CHINA',    265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_rice+CHINA_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(155) = 1,  'months', 'first',0, 'Mfx_ri_EU',       265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_rice+EU_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(156) = 1,  'months', 'first',0, 'Mfx_ri_INDIA',    265,1,276,1,
```

```
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_rice+INDIA_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(157) = 1,  'months', 'first',0, 'Mfx_ri_NA',       265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_rice+NA_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(158) = 1,  'months', 'first',0, 'Mfx_ri_SA',       265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_rice+SA_CH4_199001-201212.nml; VAR=CH4;',
!
! termites
!
RG_TRIG(159) = 1,  'months',  'first',0, 'Mfx_te',         265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_biotermites_CH4_199001-201212.nml; VAR=CH4;',
!
! volcanoes
!
RG_TRIG(160) = 1,  'months',  'first',0, 'Mfx_vo',         265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_volc_CH4_199001-201212.nml; VAR=CH4;',
!
! wetlands
!
RG_TRIG(161) = 1,  'months', 'first',0, 'Mfx_wl_AUS',     265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_biowetlands+AUS_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(162) = 1,  'months', 'first',0, 'Mfx_wl_CHINA',   265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_biowetlands+CHINA_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(163) = 1,  'months', 'first',0, 'Mfx_wl_EU',      265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_biowetlands+EU_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(164) = 1,  'months', 'first',0, 'Mfx_wl_india',   265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_biowetlands+INDIA_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(165) = 1,  'months', 'first',0, 'Mfx_wl_MIDEAST', 265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_biowetlands+MIDEAST_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(166) = 1,  'months', 'first',0, 'Mfx_wl_NA_bor',  265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_biowetlands+NAbor_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(167) = 1,  'months', 'first',0, 'Mfx_wl_N_AFR',   265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_biowetlands+NAFR_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(168) = 1,  'months', 'first',0, 'Mfx_wl_NA_TEMP', 265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_biowetlands+NAtemp_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(169) = 1,  'months', 'first',0, 'Mfx_wl_RUS',     265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_biowetlands+RUS_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(170) = 1,  'months', 'first',0, 'Mfx_wl_S_AFR',   265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_biowetlands+SAFR_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(171) = 1,  'months', 'first',0, 'Mfx_wl_SA_temp', 265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_biowetlands+SAtemp_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(172) = 1,  'months', 'first',0, 'Mfx_wl_SA_TROP', 265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_biowetlands+SAtrop_CH4_199001-201212.nml; VAR=CH4;',
RG_TRIG(173) = 1,  'months', 'first',0, 'Mfx_wl_se_asia', 265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_biowetlands+SEASIA_CH4_199001-201212.nml; VAR=CH4;',
```

```
!
! wild animals
!
RG_TRIG(174) = 1,   'months',  'first',0, 'Mfx_wa',         265,1,276,1,
        'NML=./import/offemis/CH4/EMPA/EMPA_DLR1.1_PostE_wildlife_CH4_199001-201212.nml; VAR=CH4;',
!
```

3.4 OFFEMIS

Namelist 6. Example of the offemis.nml, which couples the imported emissions to the master CH_4 tracer `CH4_fx`, to the isotopologues, scaled according to the emission signature, and to the corresponding emission class tracers.

```
! ### SYNTAX:
!     (SPECIFIERS MUST BE UPPERCASE !)
! ###         GP=    Gridpoint  Emission Method (0,1,2) (SURFACE ONLY)
!                    0: no emission; only channel object (DEFAULT)
!                    1: 2D (SURFACE EM.) -> lowest layer
!                       3D (VOLUME  EM.) -> emission ON
!                       Nx2D (MULTI LEVEL EM.) -> internally converted to 3D
!                    SURFACE EMISSIONS ONLY:
!                    2: lower boundary condition for flux
!
! ###         LG=    Lagrangian Emission Method (0,1,2,3,4)
!                    0: no emission; only channel object (DEFAULT)
!                    1: 2D (SURFACE EM.)       -> into CELLs in lowest layer
!                       3D (VOLUME  EM.)       -> emission ON
!                       Nx2D (MULTI LEVEL EM.) -> internally converted to 3D
!                    SURFACE EMISSIONS ONLY:
!                    2: into lowest CELLs within boundary layer
!                    3: into all CELLs in boundary layer (vertical gradient)
!                    4: into all CELLs in boundary layer (no vertical gradient)
!
!NOTEs:  (1) Surface emission fluxes (2D) must be in  molecules m-2 s-1.
!        (2) Volume emissions (3D)        must be in  molecules m-3 s-1.
!        (3) Multi level emissions (Nx2D) must be in  molecules m-2 s-1.
!        (4) For volume emissions (3D), the corresponding channel object
!            must be in the GP_3D_MID representation
!        (5) The trigger for multi level emissions (Nx2D) is the presence
!            of the channel object attribute heights
!
! EMISSION: 'TRACER[_SUBNAME][,scaling];...', CHANNEL NAME, CHANNEL OBJECT,
!           EMISSION METHOD
!
! LOWER BOUNDARY CONDITIONS (SEE tnudge.nml)
```

```
!
! ###########################################
! DIRECT EMISSIONS
! ###########################################
!
EMIS_IN(190) = ’CH4_fx;CH4_12C,0.9894892;CH4_13C,0.0105108;CH4_D0,0.9995110;CH4_D1,0.0004890;CH4_fx_e01_a01’,
                                                          ’import_grid’, ’Mfx_an_AFRICA_CH4’, ’GP=2’, ! anth.
EMIS_IN(191) = ’CH4_fx;CH4_12C,0.9894892;CH4_13C,0.0105108;CH4_D0,0.9995110;CH4_D1,0.0004890;CH4_fx_e02_a01’,
                                                          ’import_grid’, ’Mfx_an_AUS_CH4’, ’GP=2’, ! anth.
EMIS_IN(192) = ’CH4_fx;CH4_12C,0.9894892;CH4_13C,0.0105108;CH4_D0,0.9995110;CH4_D1,0.0004890;CH4_fx_e03_a01’,
                                                          ’import_grid’, ’Mfx_an_CHINA_CH4’, ’GP=2’, ! anth.
EMIS_IN(193) = ’CH4_fx;CH4_12C,0.9894892;CH4_13C,0.0105108;CH4_D0,0.9995110;CH4_D1,0.0004890;CH4_fx_e04_a01’,
                                                          ’import_grid’, ’Mfx_an_EU_CH4’, ’GP=2’, ! anth.
EMIS_IN(194) = ’CH4_fx;CH4_12C,0.9894892;CH4_13C,0.0105108;CH4_D0,0.9995110;CH4_D1,0.0004890;CH4_fx_e05_a01’,
                                                          ’import_grid’, ’Mfx_an_INDIA_CH4’, ’GP=2’, ! anth.
EMIS_IN(195) = ’CH4_fx;CH4_12C,0.9894892;CH4_13C,0.0105108;CH4_D0,0.9995110;CH4_D1,0.0004890;CH4_fx_e06_a01’,
                                                          ’import_grid’, ’Mfx_an_MIDEAST_CH4’, ’GP=2’, ! anth.
EMIS_IN(196) = ’CH4_fx;CH4_12C,0.9894892;CH4_13C,0.0105108;CH4_D0,0.9995110;CH4_D1,0.0004890;CH4_fx_e07_a01’,
                                                          ’import_grid’, ’Mfx_an_NA_CH4’, ’GP=2’, ! anth.
EMIS_IN(197) = ’CH4_fx;CH4_12C,0.9894892;CH4_13C,0.0105108;CH4_D0,0.9995110;CH4_D1,0.0004890;CH4_fx_e08_a01’,
                                                          ’import_grid’, ’Mfx_an_OCEAN_CH4’, ’GP=2’, ! anth.
EMIS_IN(198) = ’CH4_fx;CH4_12C,0.9894892;CH4_13C,0.0105108;CH4_D0,0.9995110;CH4_D1,0.0004890;CH4_fx_e09_a01’,
                                                          ’import_grid’, ’Mfx_an_RUS_CH4’, ’GP=2’, ! anth.
EMIS_IN(199) = ’CH4_fx;CH4_12C,0.9894892;CH4_13C,0.0105108;CH4_D0,0.9995110;CH4_D1,0.0004890;CH4_fx_e10_a01’,
                                                          ’import_grid’, ’Mfx_an_SA_CH4’, ’GP=2’, ! anth.
EMIS_IN(200) = ’CH4_fx;CH4_12C,0.9894892;CH4_13C,0.0105108;CH4_D0,0.9995110;CH4_D1,0.0004890;CH4_fx_e11_a01’,
                                                          ’import_grid’, ’Mfx_an_SE_ASIA_CH4’, ’GP=2’, ! anth.
!
! biomass burning
!
EMIS_IN(201) = ’CH4_fx;CH4_12C,0.9892048;CH4_13C,0.0107952;CH4_D0,0.9995097;CH4_D1,0.0004903;CH4_fx_e12_a01’,
                                                          ’import_grid’, ’BB_AUS_CH4’,     ’GP=2’, ! bb
EMIS_IN(202) = ’CH4_fx;CH4_12C,0.9892048;CH4_13C,0.0107952;CH4_D0,0.9995097;CH4_D1,0.0004903;CH4_fx_e13_a01’,
                                                          ’import_grid’, ’BB_CHINA_CH4’,     ’GP=2’, ! bb
EMIS_IN(203) = ’CH4_fx;CH4_12C,0.9892048;CH4_13C,0.0107952;CH4_D0,0.9995097;CH4_D1,0.0004903;CH4_fx_e14_a01’,
                                                          ’import_grid’, ’BB_EU_CH4’,     ’GP=2’, ! bb
EMIS_IN(204) = ’CH4_fx;CH4_12C,0.9892048;CH4_13C,0.0107952;CH4_D0,0.9995097;CH4_D1,0.0004903;CH4_fx_e15_a01’,
                                                          ’import_grid’, ’BB_INDIA_CH4’,     ’GP=2’, ! bb
EMIS_IN(205) = ’CH4_fx;CH4_12C,0.9892048;CH4_13C,0.0107952;CH4_D0,0.9995097;CH4_D1,0.0004903;CH4_fx_e16_a01’,
                                                          ’import_grid’, ’BB_NA_bor_CH4’,     ’GP=2’, ! bb
EMIS_IN(206) = ’CH4_fx;CH4_12C,0.9892048;CH4_13C,0.0107952;CH4_D0,0.9995097;CH4_D1,0.0004903;CH4_fx_e17_a01’,
                                                          ’import_grid’, ’BB_N_AFR_CH4’,     ’GP=2’, ! bb
EMIS_IN(207) = ’CH4_fx;CH4_12C,0.9892048;CH4_13C,0.0107952;CH4_D0,0.9995097;CH4_D1,0.0004903;CH4_fx_e18_a01’,
                                                          ’import_grid’, ’BB_NA_temp_CH4’,     ’GP=2’, ! bb
```

```
EMIS_IN(208) = 'CH4_fx;CH4_12C,0.9892048;CH4_13C,0.0107952;CH4_D0,0.9995097;CH4_D1,0.0004903;CH4_fx_e19_a01',
                                                            'import_grid', 'BB_N_MIDEAST_CH4',     'GP=2', ! bb
EMIS_IN(209) = 'CH4_fx;CH4_12C,0.9892048;CH4_13C,0.0107952;CH4_D0,0.9995097;CH4_D1,0.0004903;CH4_fx_e20_a01',
                                                            'import_grid', 'BB_RUS_CH4',     'GP=2', ! bb
EMIS_IN(210) = 'CH4_fx;CH4_12C,0.9892048;CH4_13C,0.0107952;CH4_D0,0.9995097;CH4_D1,0.0004903;CH4_fx_e21_a01',
                                                            'import_grid', 'BB_S_AFR_CH4',     'GP=2', ! bb
EMIS_IN(211) = 'CH4_fx;CH4_12C,0.9892048;CH4_13C,0.0107952;CH4_D0,0.9995097;CH4_D1,0.0004903;CH4_fx_e22_a01',
                                                            'import_grid', 'BB_SA_temp_CH4',     'GP=2', ! bb
EMIS_IN(212) = 'CH4_fx;CH4_12C,0.9892048;CH4_13C,0.0107952;CH4_D0,0.9995097;CH4_D1,0.0004903;CH4_fx_e23_a01',
                                                            'import_grid', 'BB_SA_trop_CH4',     'GP=2', ! bb
EMIS_IN(213) = 'CH4_fx;CH4_12C,0.9892048;CH4_13C,0.0107952;CH4_D0,0.9995097;CH4_D1,0.0004903;CH4_fx_e24_a01',
                                                            'import_grid', 'BB_SE_ASIA_CH4',     'GP=2', ! bb
!
! ocean
!
EMIS_IN(214) = 'CH4_fx;CH4_12C,0.9895891;CH4_13C,0.0104109;CH4_D0,0.9995141;CH4_D1,0.0004859;CH4_fx_e25_a01',
                                                            'import_grid', 'Mfx_oc_CH4', 'GP=2', ! ocean
!
! rice
!
EMIS_IN(215) = 'CH4_fx;CH4_12C,0.9896329;CH4_13C,0.0103671;CH4_D0,0.9995791;CH4_D1,0.0004209;CH4_fx_e26_a01',
                                                            'import_grid', 'Mfx_ri_AFR_CH4', 'GP=2', ! rice
EMIS_IN(216) = 'CH4_fx;CH4_12C,0.9896329;CH4_13C,0.0103671;CH4_D0,0.9995791;CH4_D1,0.0004209;CH4_fx_e27_a01',
                                                            'import_grid', 'Mfx_ri_ASIA_AUS_CH4', 'GP=2', ! rice
EMIS_IN(217) = 'CH4_fx;CH4_12C,0.9896329;CH4_13C,0.0103671;CH4_D0,0.9995791;CH4_D1,0.0004209;CH4_fx_e28_a01',
                                                            'import_grid', 'Mfx_ri_CHINA_CH4', 'GP=2', ! rice
EMIS_IN(218) = 'CH4_fx;CH4_12C,0.9896329;CH4_13C,0.0103671;CH4_D0,0.9995791;CH4_D1,0.0004209;CH4_fx_e29_a01',
                                                            'import_grid', 'Mfx_ri_EU_CH4', 'GP=2', ! rice
EMIS_IN(219) = 'CH4_fx;CH4_12C,0.9896329;CH4_13C,0.0103671;CH4_D0,0.9995791;CH4_D1,0.0004209;CH4_fx_e30_a01',
                                                            'import_grid', 'Mfx_ri_INDIA_CH4', 'GP=2', ! rice
EMIS_IN(220) = 'CH4_fx;CH4_12C,0.9896329;CH4_13C,0.0103671;CH4_D0,0.9995791;CH4_D1,0.0004209;CH4_fx_e31_a01',
                                                            'import_grid', 'Mfx_ri_NA_CH4', 'GP=2', ! rice
EMIS_IN(221) = 'CH4_fx;CH4_12C,0.9896329;CH4_13C,0.0103671;CH4_D0,0.9995791;CH4_D1,0.0004209;CH4_fx_e32_a01',
                                                            'import_grid', 'Mfx_ri_SA_CH4', 'GP=2', ! rice
!
! termites
!
EMIS_IN(222) = 'CH4_fx;CH4_12C,0.9896366;CH4_13C,0.0103634;CH4_D0,0.9996200;CH4_D1,0.0003800;CH4_fx_e33_a01',
                                                            'import_grid', 'Mfx_te_CH4', 'GP=2', ! termites
!
! volcanoes
!
EMIS_IN(223) = 'CH4_fx;CH4_12C,0.9893910;CH4_13C,0.0106090;CH4_D0,0.9995349;CH4_D1,0.0004651;CH4_fx_e34_a01',
                                                            'import_grid', 'Mfx_vo_CH4', 'GP=2', ! volcanoes
```

```
!
! wetlands
!
EMIS_IN(224) = 'CH4_fx;CH4_12C,0.9895934;CH4_13C,0.0104066;CH4_D0,0.9995865;CH4_D1,0.0004135;CH4_fx_e35_a01',
                                                          'import_grid', 'Mfx_wl_AUS_CH4', 'GP=2', ! wetlands
EMIS_IN(225) = 'CH4_fx;CH4_12C,0.9895934;CH4_13C,0.0104066;CH4_D0,0.9995865;CH4_D1,0.0004135;CH4_fx_e36_a01',
                                                          'import_grid', 'Mfx_wl_CHINA_CH4', 'GP=2', ! wetlands
EMIS_IN(226) = 'CH4_fx;CH4_12C,0.9895934;CH4_13C,0.0104066;CH4_D0,0.9995865;CH4_D1,0.0004135;CH4_fx_e37_a01',
                                                          'import_grid', 'Mfx_wl_EU_CH4', 'GP=2', ! wetlands
EMIS_IN(227) = 'CH4_fx;CH4_12C,0.9895934;CH4_13C,0.0104066;CH4_D0,0.9995865;CH4_D1,0.0004135;CH4_fx_e38_a01',
                                                          'import_grid', 'Mfx_wl_india_CH4', 'GP=2', ! wetlands
EMIS_IN(228) = 'CH4_fx;CH4_12C,0.9895934;CH4_13C,0.0104066;CH4_D0,0.9995865;CH4_D1,0.0004135;CH4_fx_e39_a01',
                                                          'import_grid', 'Mfx_wl_MIDEAST_CH4', 'GP=2', ! wetlands
EMIS_IN(229) = 'CH4_fx;CH4_12C,0.9895934;CH4_13C,0.0104066;CH4_D0,0.9995865;CH4_D1,0.0004135;CH4_fx_e40_a01',
                                                          'import_grid', 'Mfx_wl_NA_bor_CH4', 'GP=2', ! wetlands
EMIS_IN(230) = 'CH4_fx;CH4_12C,0.9895934;CH4_13C,0.0104066;CH4_D0,0.9995865;CH4_D1,0.0004135;CH4_fx_e41_a01',
                                                          'import_grid', 'Mfx_wl_N_AFR_CH4', 'GP=2', ! wetlands
EMIS_IN(231) = 'CH4_fx;CH4_12C,0.9895934;CH4_13C,0.0104066;CH4_D0,0.9995865;CH4_D1,0.0004135;CH4_fx_e42_a01',
                                                          'import_grid', 'Mfx_wl_NA_TEMP_CH4', 'GP=2', ! wetlands
EMIS_IN(232) = 'CH4_fx;CH4_12C,0.9895934;CH4_13C,0.0104066;CH4_D0,0.9995865;CH4_D1,0.0004135;CH4_fx_e43_a01',
                                                          'import_grid', 'Mfx_wl_RUS_CH4', 'GP=2', ! wetlands
EMIS_IN(233) = 'CH4_fx;CH4_12C,0.9895934;CH4_13C,0.0104066;CH4_D0,0.9995865;CH4_D1,0.0004135;CH4_fx_e44_a01',
                                                          'import_grid', 'Mfx_wl_S_AFR_CH4', 'GP=2', ! wetlands
EMIS_IN(234) = 'CH4_fx;CH4_12C,0.9895934;CH4_13C,0.0104066;CH4_D0,0.9995865;CH4_D1,0.0004135;CH4_fx_e45_a01',
                                                          'import_grid', 'Mfx_wl_SA_temp_CH4', 'GP=2', ! wetlands
EMIS_IN(235) = 'CH4_fx;CH4_12C,0.9895934;CH4_13C,0.0104066;CH4_D0,0.9995865;CH4_D1,0.0004135;CH4_fx_e46_a01',
                                                          'import_grid', 'Mfx_wl_SA_TROP_CH4', 'GP=2', ! wetlands
EMIS_IN(236) = 'CH4_fx;CH4_12C,0.9895934;CH4_13C,0.0104066;CH4_D0,0.9995865;CH4_D1,0.0004135;CH4_fx_e47_a01',
                                                          'import_grid', 'Mfx_wl_se_asia_CH4', 'GP=2', ! wetlands
!
! wild animals
!
EMIS_IN(237) = 'CH4_fx;CH4_12C,0.9896165;CH4_13C,0.0103835;CH4_D0,0.9995758;CH4_D1,0.0004242;CH4_fx_e48_a01',
                                                          'import_grid', 'Mfx_wa_CH4', 'GP=2', !wild animals
```

3.5 TNUDGE

Namelist 7. Example entries to nudge the tracers `CH4` and `CH4_fx` to a predefined lower boundary condition.

```
!# SYNTAX:
!#          tracer, subname, channel, object, nudging-coeff. [s],
!#          min.lat, max.lat, min.lev, max.lev, min.lon, max.lon,
!#          flux diagnostic ?
!# NOTES:
```

```
!#   - special levels: -3 boundary layer ,-2 tropopause, -1 top, 0 surface
!#   - nudging-coeff < 0: apply 'hard' nudging with coeff = model time step
!#
! GHG
TNUDGE_GP(2)  = 'CH4','',     'import_grid','TN_GHG_CH4',10800.0,-90.0,90.0,0,0,0.0,360.0,T,'','','','',0,
!
TNUDGE_GP(4)  = 'CH4','fx',   'import_grid','TN_GHG_CH4',10800.0,-90.0,90.0,0,0,0.0,360.0,T,'','','','',0,
!
```

3.6 H2OISO

Namelist 8. Namelist of the submodel H2OISO as used in the presented examples.

```
&CTRL
/
&CPL
l_steady = T          ! start from steady-state conditions
                      ! this means q, xl and xi are initialized by
                      ! H2OISOHHOvap, H2OISOHHOliq and H2OISOHHOice,
                      ! which are initialized via tracer.nml
l_noconvect_dd = F    ! set true only for sensitivity study
                      ! without influence of convect on deltaD
l_nocloud_dd   = F    ! set true only for sensitivity study
                      ! without influence of cloud on deltaD
/
```

4 Isotopic signatures of emission sources

Table S1. Flux in [$\times 10^{12}$ g CH_4 per year (Tg CH_4 a^{-1})] and signatures in [‰] of CH_4 sources. Flux values are taken from the IPCC (2013) bottom-up estimate for 2000-2009. Signatures of bulk source types (other natural, agriculture & waste, and fossil fuel) are averages weighted by the individual flux strength contributions.

		signature of ^{13}C in CH_4 ($\delta^{13}C(CH_4)$)			signature of D in CH_4 ($\delta D(CH_4)$)			
source	flux	δ-value	±	ref.	δ-value	±	ref.	type
wetlands	**217**	**-59.4**	**1.5**	1,2,3,4,6	**-336.2**	**23.8**	3,4,6	biogenic
other natural	**126**	**-50.3**	**8.9**		**-313.3**	**88.9**		
freshwater	40	-53.8	/	3	-385.0	/	3	biogenic
wildanimals	15	-61.5	0.5	1	-319.0	/	5	biogenic
termites	11	-63.3	6.5	1,2,3	-390.0	35.5	3	biogenic
volcanoes	54	-40.9	0.9	1,2	-253.4	53.4	3,7	fossil
ocean/hydrates	6	-59.0	1.0	1,2,3	-220.0	/	3	biogenic
agriculture & waste	**200**	**-57.5**	**3.8**		**-313.8**	**26.5**		
ruminants	89	-60.2	0.3	3,4,6	-317.5	12.5	3,4	biogenic
landfills	75	-51.7	2.5	3,4,6	-304.3	8.5	3,4,6	biogenic
rice	36	-63.0	1.0	1,2,3,4,6	-324.3	5.5	3,4,6	biogenic
fossil fuel	**96**	**-41.8**	**7.5**		**-154.2**	**2.5**		
natural gas	32	-43.5	0.5	3,6	-182.5	2.5	3,6	fossil
coal	64	-41.0	7.0	3,6,8	-140.0	0.0	3,6	fossil
biomass burning	**35**	**-23.9**	**1.6**	1,2,3,4,6	**-213.0**	**7.5**	3,4,6	pyrogenic
biogenic		-59.0			-324.5			
fossil		-41.8			-192.0			
pyrogenic		-23.9			-213.0			

references: (1) (Monteil et al., 2011) (2) (Fletcher et al., 2004) (3) (Whiticar and Schaefer, 2007) (4) (Snover and Quay, 2000) (5) (Rigby et al., 2012) (6) (Quay et al., 1999) (7) (Kiyosu, 1983) (8) (Zazzeri et al., 2015)

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