

**Supplementary material to the article
“Contribution of emissions to concentrations: The
TAGGING 1.0 submodel based on the Modular Earth
Submodel System (MESSy 2.52)”, Geosci. Model Dev.
Disc. (2016), including the documentation of the submodel
TAGGING 1.0 and the tool ProdLoss 1.1**

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1 Introduction

This documentation provides supplementary material to the above mentioned article. It provides a brief overview on the used present-day simulation and gives an overview on the EMAC submodel TAGGING (Section 3) and the tool ProdLoss (Section 4). The submodel TAGGING calculates the contribution of emissions to atmospheric concentrations of ozone, and other species and families. The tool ProdLoss identifies in a given set of reactions, i.e. a chemical mechanism, reactions which produce or destroy a given chemical family.

2 Comparison with RC1SD-base10a

The Figures 1 to 4 show a comparison of temperature, CO, NO_x and O₃ between the RC1SD-base10a described by Jöckel et al. (2016) and the simulation performed here (RC1SD-base10a_tag). The simulation set-up differs by use of the TAGGING submodel and the QCTM-mode (Deckert et al., 2011). The simulations show only minor differences.

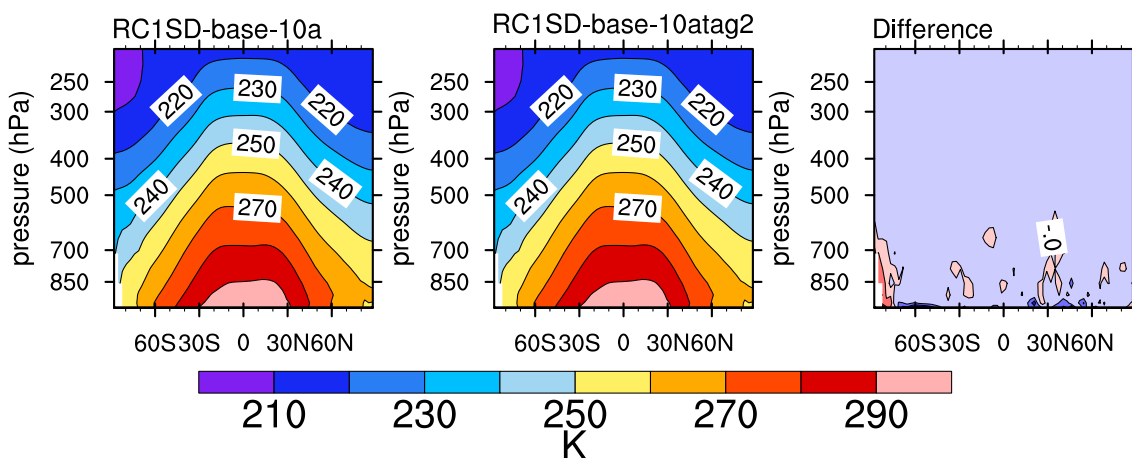


Figure 1: Zonally averaged annual mean temperature (in K) for the time period 2005 to 2010. The left plot shows the value for the RC1SD-base10a, the middle plot the value for the simulation RC1SD-base10a_tag and the right plot the absolute difference between the two fields. The colour bar indicates only the values for the first two plots.

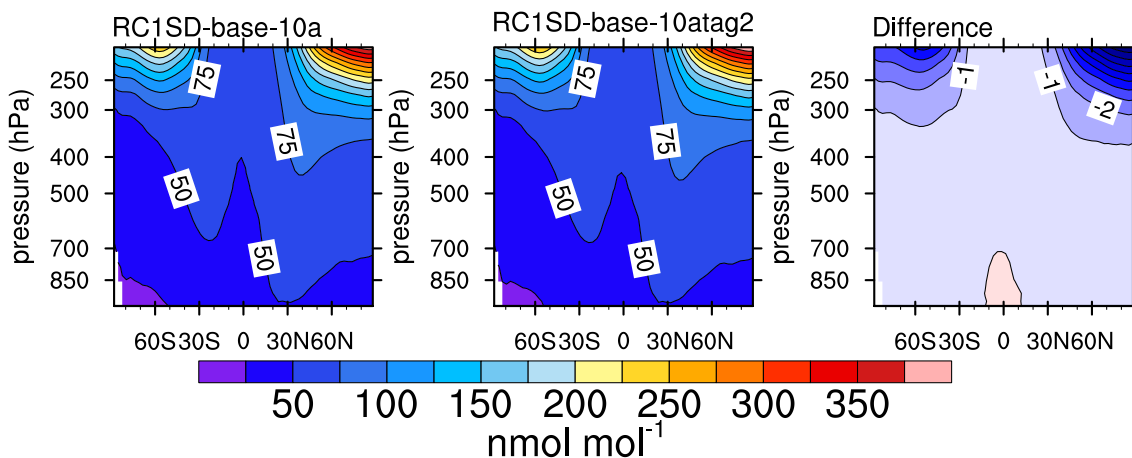


Figure 2: As Fig. 1 but for O₃ (in nmol/mol).

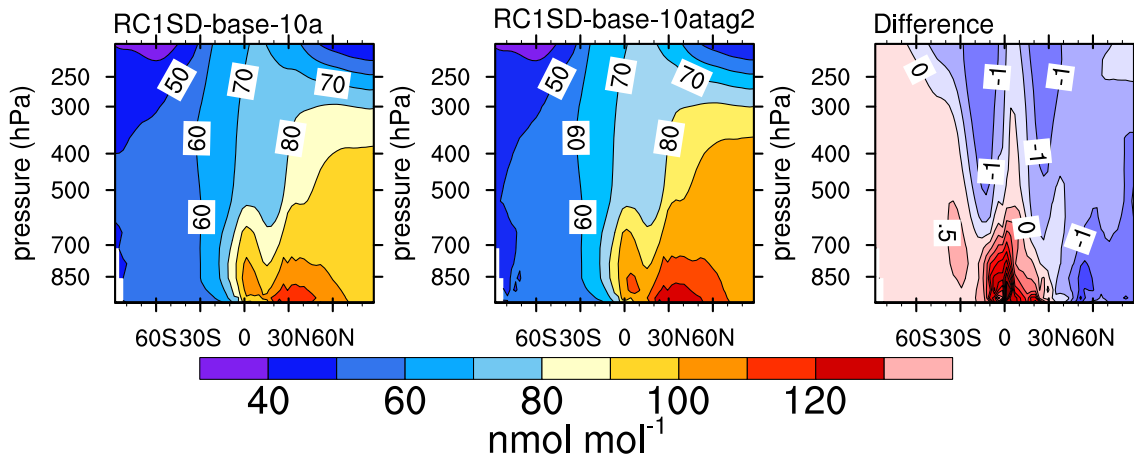


Figure 3: As Fig. 1 but for CO (in nmol/mol).

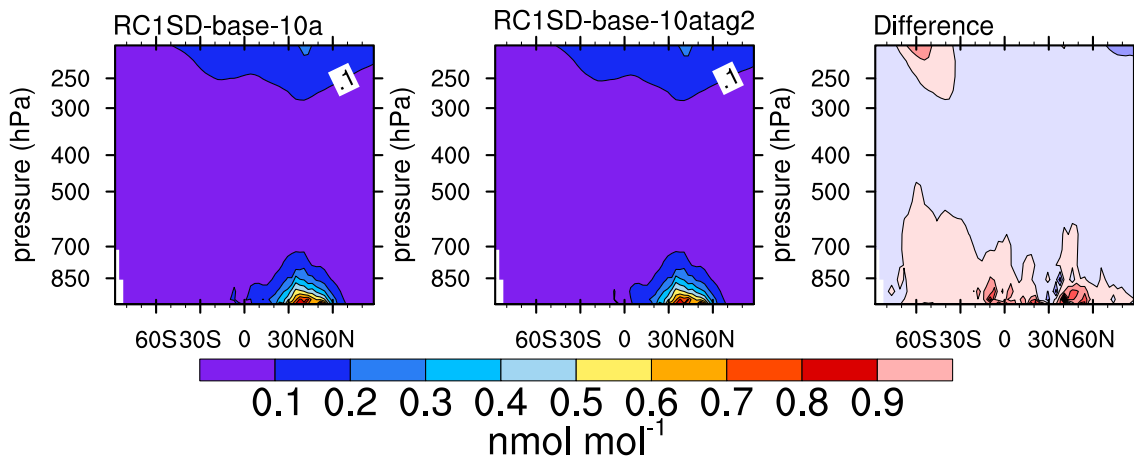


Figure 4: As Fig. 1 but for NO_x (in nmol/mol).

Table 1: Overview on the families NO_y, NMHC, and O₃.

NO _y		NMHC		ODD	
weight: 1					
N	NO	CH ₃ OH	CH ₃ O ₂	O ₃	O(³ P)
NO ₂	NO ₃	CH ₃ OOH	HCHO	O(¹ D)	ClO
HONO	HNO ₃	HCOOH		HOCl	OCIO
HNO ₄	NACA			NO ₂	HNO ₃
MPAN	IC ₃ H ₇ NO ₃			HNO ₄	PAN
LC ₄ H ₉ NO ₃	ISON			NACA	MPAN
ClNO ₃	BrNO ₃			IC ₃ H ₇ NO ₃	LC ₄ H ₉ NO ₃
				ISON	BrO
				ClO	
weight: 2					
N ₂ O ₅		C ₂ H ₆	C ₂ H ₄	Cl ₂ O ₂	NO ₃
		C ₂ H ₅ O ₂	C ₂ H ₅ OOH	ClONO ₂	BrONO ₂
		CH ₃ CHO	CH ₃ CO ₂ H		
		CH ₃ CO ₃	CH ₃ CO ₃ H		
		NACA			
weight: 3					
		C ₃ H ₈	C ₃ H ₆	N ₂ O ₅	
		IC ₃ H ₇ O ₂	IC ₃ H ₇ OOH		
		LHOC ₃ H ₆ O ₂	LHOC ₃ H ₆ OOH		
		CH ₃ COCH ₃	CH ₃ COCH ₂ O ₂		
		HYPERACET	ACETOL		
		MYGLYOX	MPAN		
		IC ₃ H ₇ NO ₃			
weight: 4					
		NC ₄ H ₁₀	LC ₄ H ₉ O ₂		
		LC ₄ H ₉ OOH	MVK		
		MVKO ₂	MVKOOH		
		MEK	LMEKO ₂		
		LMEKOOH	BIACET		
		LC ₄ H ₉ NO ₃			
weight: 5					
		C ₅ H ₈	ISO ₂		
		ISOOH	ISON		

3 The submodel TAGGING

3.1 Families

The tagging scheme employs a simplified chemical scheme, which is derived from the standard MECCA set-up. This scheme includes the species O₃, PAN, CO, OH, HO₂, and two families NO_y, lumping all short-lived nitrogen compounds except PAN and NMHC, lumping all non-methane hydrocarbons. PAN is treated separately to account for long-range transport of nitrogen compounds in the upper troposphere.

The reaction rates for production and loss processes are derived from MECCA (Sander et al., 2011), by using its diagnostic package for reaction rates. The tool *ProdLoss* is used to identify the relevant reactions and number of produced molecules of families.

3.2 General structure

The structure of the submodel TAGGING follows the MESSy2 coupling standards (Jöckel et al., 2010). Note that using the variable `time_step_len` from the submodel *TIMER* gives automatically the correct integration time, which is *dt* for Runge Kutta and *2 dt* for leap frog.

<i>Submodel Interface Layer</i>	<i>Base Model Core Layer</i>
<code>messy_tagging_si.f90</code>	<code>messy_tagging.f90</code>
<code>tagging_initialize</code> Calls subroutines to read CTRL and CPL namelists	
<code>tagging_read_nml_cpl</code> Reads coupling relevant parameters	<code>tagging_read_nml_ctrl</code> Reads core relevant parameters
<code>tagging_new_tracer</code> Definition of TAGGING tracers	
<code>tagging_init_memory</code> Allocation of fields and generation of TAGGING channel objects	
<code>tagging_init_coupling</code> Initialise coupling, makes information available from other submodels	
<code>tagging_init_tracer</code> Initialisation of TAGGING tracers, e.g. from restart files or using	
<code>tagging_init_tracer_online</code> Online initialisation of tracers in the case of simulation from scratch.	
<code>tagging_local_start</code> Store X0 values for chemical fields after transport	
<code>tagging_vdiff</code> Compares pre- and after vdiff tendencies of tracers to account for on-line emissions of tracers	
<code>tagging_physc</code> First calculate X1 values, then calculate chemical changes	<code>tagging_tendencies</code> Adapt Production and Loss terms to the chosen tagging integration scheme
	<code>tagging_get_HOx_tendencies</code> Solves equation to get HOx tendencies
	<code>tagging_get_tendencies</code> Re-Calculate the production and loss terms of the C-compounds based on MECCA output
	<code>tagging_chemistry</code> Calculate impact of emissions on short-lived species
<code>tagging_free_memory</code> Release memory	

3.3 The subroutine `tagging_tendencies`

ELEMENTAL SUBROUTINE <code>tagging_tendencies</code>			
name	type	intent	description
mandatory arguments:			
<i>General information</i>			
<code>kproma</code>	REAL(DP)	IN	dimension <code>kproma</code> of input fields
<code>nlev</code>	REAL(DP)	IN	dimension <code>nlev</code> of input fields
<code>dt</code>	REAL(DP)	IN	time step in seconds
<code>X1</code>	REAL(DP)	IN	species at timestep X1 [mol/mol]
<code>X2</code>	REAL(DP)	IN	species at timestep X2 [mol/mol]
<code>P</code>	REAL(DP)	IN	production rate of species [mol/mol/s]
<code>D</code>	REAL(DP)	IN	loss rate of species [mol/mol/s]
<code>alpha</code>	REAL(DP)	OUT	correction factor ≥ 0
<code>beta</code>	REAL(DP)	OUT	correction factor ≥ 0

3.4 The subroutine tagging_HOx_tendencies

ELEMENTAL SUBROUTINE tagging_HOx_tendencies			
name	type	intent	description
mandatory arguments:			
<i>General information</i>			
kproma	REAL(DP)	IN	dimension kproma of input fields
nlev	REAL(DP)	IN	dimension nlev of input fields
dt	REAL(DP)	IN	time step in seconds
OH	REAL(DP)	IN	species at timestep X1 [mol/mol]
HO2	REAL(DP)	IN	species at timestep X2 [mol/mol]
P	REAL(DP)	IN	production rate of species [mol/mol/s]
D1	REAL(DP)	IN	loss rate of specie [mol/mol/s]
D2	REAL(DP)	IN	loss rate of specie [mol/mol/s]
alpha	REAL(DP)	OUT	correction factor ≥ 0
beta	REAL(DP)	OUT	correction factor ≥ 0
gamma	REAL(DP)	OUT	correction factor ≥ 0

3.5 The subroutine tagging_get_tendencies

ELEMENTAL SUBROUTINE tagging_get_tendencies			
name	type	intent	description
mandatory arguments:			
<i>General information</i>			
kproma	REAL(DP)	IN	dimension kproma of input fields
nlev	REAL(DP)	IN	dimension nlev of input fields
dt	REAL(DP)	IN	time step in seconds
ch4_1	REAL(DP)	IN	CH4 before MECCA [mol/mol]
ch4_2	REAL(DP)	IN	CH4 after MECCA [mol/mol]
co_1	REAL(DP)	IN	CO before MECCA [mol/mol]
co_2	REAL(DP)	IN	CO after MECCA [mol/mol]
pan_1	REAL(DP)	IN	PAN before MECCA [mol/mol]
pan_2	REAL(DP)	IN	PAN after MECCA [mol/mol]
nmhc_1	REAL(DP)	IN	NMHC before MECCA [mol/mol]
nmhc_2	REAL(DP)	IN	NMHC after MECCA [mol/mol]
ch4loss	REAL(DP)	OUT	calculated CH4 loss rate [mol/mol/s]
coprod	REAL(DP)	OUT	calculated CO production rate [mol/mol/s]
coloss	REAL(DP)	OUT	calculated CO loss rate [mol/mol/s]

3.6 The subroutine tagging_chemistry

ELEMENTAL SUBROUTINE tagging_chemistry			
name	type	intent	description
mandatory arguments:			
<i>General information</i>			
ngpblks kproma	REAL(DP)	IN	dimension kproma of input fields
nlev	REAL(DP)	IN	dimension nlev of input fields
dt	REAL(DP)	IN	time step in seconds
o3_tagging	REAL(DP)	IN	mixing ratios o3_tagging tracers [mol/mol]
noy_tagging	REAL(DP)	IN	mixing ratios noy_tagging tracers [mol/mol]
nmhc_tagging	REAL(DP)	IN	mixing ratios nmhc_tagging tracers [mol/mol]
co_tagging	REAL(DP)	IN	mixing ratios co_tagging tracers [mol/mol]
co_tagging_sum	REAL(DP)	IN	sum of mixing ratios for co_tagging tracer over all categories [mol/mol]
nmhc_tagging_sum	REAL(DP)	IN	sum of mixing ratios for nmhc_tagging tracer over all categories [mol/mol]
noy_tagging_sum	REAL(DP)	IN	sum of mixing ratios for noy_tagging tracer over all categories [mol/mol]
o3_tagging_sum	REAL(DP)	IN	sum of mixing ratios for o3_tagging tracer over all categories [mol/mol]
pan_tagging_sum	REAL(DP)	IN	sum of mixing ratios for pan_tagging tracer over all categories [mol/mol]
oh oh	REAL(DP)	IN	OH tendency [mol/mol/s]
ho2	REAL(DP)	IN	HO2 tendency [mol/mol/s]
do3	REAL(DP)	IN	o3 tag tendency [mol/mol/s]
dnoy	REAL(DP)	IN	noy tag tendency [mol/mol/s]
dpan	REAL(DP)	IN	pan tag tendency [mol/mol/s]
dnmhc	REAL(DP)	IN	nmhc tag tendency [mol/mol/s]
dco	REAL(DP)	IN	co tag tendency [mol/mol/s]
lossOH	REAL(DP)	IN	tendency lossOH tracer [mol/mol/s]
oh_2	REAL(DP)	IN	OH mixing ratio at timestep 2
ho_2	REAL(DP)	IN	HO2 mixing ratio at timestep 2
ch4_2	REAL(DP)	IN	CH4 mixing ratio at timestep 2
oh_tag	REAL(DP)	INOUT	tagged OH mixing ratio
ho2_tag	REAL(DP)	INOUT	tagged HO2 mixing ratio
o3prod_ho2	REAL(DP)	IN	tendency of o3prodho2 tracer [mol/mol/s]
o3prod_ro2	REAL(DP)	IN	tendency of o3prodho2 tracer [mol/mol/s]
o3prod_o2	REAL(DP)	IN	tendency of o3prodo2 tracer [mol/mol/s]
o3loss_oh	REAL(DP)	IN	tendency of o3lossoh tracer [mol/mol/s]
o3loss_ho2	REAL(DP)	IN	tendency of o3lossho2 tracer [mol/mol/s]
o3loss_ro	REAL(DP)	IN	tendency of o3lossro tracer [mol/mol/s]
o3loss_no	REAL(DP)	IN	tendency of o3lossno tracer [mol/mol/s]
o3loss_xo	REAL(DP)	IN	tendency of o3lossxo tracer [mol/mol/s]
o3loss	REAL(DP)	IN	tendency of o3loss tracer [mol/mol/s]
o3prod	REAL(DP)	IN	tendency of o3prod tracer [mol/mol/s]

panprod	REAL(DP)	IN	tendency of panprod tracer [mol/mol/s]
panloss	REAL(DP)	IN	tendency of panloss tracer [mol/mol/s]
coprod	REAL(DP)	IN	tendency of coprod tracer [mol/mol/s]
coloss	REAL(DP)	IN	tendency of coloss tracer [mol/mol/s]
ch4loss	REAL(DP)	IN	tendency of ch4loss tracer [mol/mol/s]
prodho2	REAL(DP)	IN	tendency of prodho2 tracer [mol/mol/s]
losso1d	REAL(DP)	IN	tendency of losso1d tracer [mol/mol/s]
noprodho2	REAL(DP)	IN	tendency of noprodho2 tracer [mol/mol/s]
ho2loss	REAL(DP)	IN	tendency of ho2loss tracer [mol/mol/s]
ohlossno2	REAL(DP)	IN	tendency of ohlossno2 tracer [mol/mol/s]
lossho2oh	REAL(DP)	IN	tendency of lossho2oh tracer [mol/mol/s]
ho2lossHO2	REAL(DP)	IN	tendency of ho2lossHO2 tracer [mol/mol/s]
po3_ho2	REAL(DP)	OUT	PO3HO2 production rate [mol/mol/s]
po3_ro2	REAL(DP)	OUT	PO3RO2 production rate [mol/mol/s]
do3_ro	REAL(DP)	OUT	PO3RO production rate [mol/mol/s]
do3_oh	REAL(DP)	OUT	DO3OH production rate [mol/mol/s]
do3_ho2	REAL(DP)	OUT	DO3HO2 production rate [mol/mol/s]
do3_xo	REAL(DP)	OUT	DO3XO production rate [mol/mol/s]
do3_no	REAL(DP)	OUT	PO3NO production rate [mol/mol/s]

3.7 Namelist

The TAGGING submodel has a control and a coupling namelist

```
! -*- f90 -*-
&CTRL
! i_tracer_init
! 0 -> tagging tracer read from restart file
! 1 -> tagging tracer reinitialised after restart
i_tracer_init=0 !-1
!l_adv_err_diag
! Additional error diagnostics if set to true
l_adv_err_diag= .false.
! i_species ! Note that OH, HO2 changes are calculated but not used for tagging chemistry for 0-2
! Tagging method (only 3 available so far)
! -0: NOy,O3 prod only
! -1: NOy,O3
! -2: NOy, CO, PAN, NMHC, O3
! -3: NOy, CO, PAN, NMHC, O3, HO2 and OH (default)
i_species=3
/
&CPL
! NOTES:
!c_lnox
!lightning nox channel and object
c_lnox = 'lnox_Grewe_gp', 'telnox'
!i_diag
! additional output
! i_diag -0 no additional output
! -1 additional output (default)
!i_diag = 1
/
```

The variables

- `i_tracer_init` determines the restart behaviour. Option 0 initialises the tracer from a restart file (in case of a restarted simulation) or can be initialised via the tracer namelist. With option 1 the TAGGING tracers are reinitialised after every restart using `tagging_init_tracer_online`.
- `l_adv_err_diag` activates additional tracer for error diagnostics
- `i_species` chooses the tagged species, however until now only option 3 is available (and default)
- `c_lnox` lightning NO_x channel and object
- `i_diag` additional output is enabled (1) or disabled (0).

Table 3: Overview of the emission classes.

Tagged sector	emission files	description
Anthropogenic non-traffic	CCMI_DLR1.0_AR5-RCP8.5_land-road-awb_aerosol_195001-201012.nc	All anthropogenic sources except traffic and AWB
Road traffic	CCMI_DLR1.0_AR5-RCP8.5_road_MISC_195001201012.nc	Road traffic emissions
Aviation	CCMI_DLR1.0_AR5-RCP8.5_air_NOx_195001201012.nc	Aviation emissions
Shipping	CCMI_DLR1.0_AR5-RCP8.5_ship_MISC_195001201012.nc	Shipping emissions
Biomass Burning	CCMI_DLR1.0_REFC1_bb_MISC_195001201012.nc CCMI_DLR1.0_REFC1_bb_NMHC_195001-201012.nc	Biomass Burning emissions
Biogenic	CCMI_DLR1.0_AR5-RCP8.5_awb_MISC_195001201012.nc GEIA_MPIC1.0_X_bio_MISC_200001_200012.nc	Biogenic and AWB

3.8 Distribution of emission classes to the tagged species

Table 3 lists the offline emission files and their corresponding tags. In addition to this the online calculated sources of soil NO_x and biogenic isoprene are summarised in the sector "biogenic". For lightning NO_x a separate sector exists.

4 The tool ProdLoss

4.1 General structure

The purpose of the tool `ProdLoss` is to provide a list of chemical reactions (including relevant reaction rates) for a chemical family. The input to `ProdLoss` is hence a definition of the chemical family (via `namelist`) and a reaction mechanism, i.e. a file describing the chemical mechanism (e.g. `gas.eqn` and `mecca.eqn`). The output file (`diagtrac.tex`) can directly be used as input for the diagnostics part of the chemical submodel MECCA (Sander et al., 2010).

4.2 Namelist

The `ProdLoss` tool has a control `namelist`. The example given below represents effective ozone production and loss terms.

```
!  -*- f90 -*-
&chempl
!  input file with reaction mechanism
infile = "gas.eqn",
!  Name of diagnostic output file will have the extension ".tex"
outfile = "diag",
!  Composition of the family with naming from infile mechanism
fam(1:22) = "O3", "O3P", "O1D", "ClO", "HOCl", "Cl2O2", "OC1O",
"NO2", "HNO3", "NO3", "N2O5", "HNO4", "PAN", "NACA",
"MPAN", "IC3H7NO3", "LC4H9NO3", "ISON", "ClNO3", "BrO", "HOBr",
"BrNO3",
!  Weights of the family members.
fac(1:22) = 1., 1., 1., 1., 1., 2., 1.,
1., 1., 2., 3., 1., 1., 1.,
1., 1., 1., 1., 2., 1., 1.,
2.,
!  Name of family.
cfam = "O3",
!  Version of MECCA
mecca = 2
/
```

The `namelist` has the following variables:

- `infile`: String of maximum `nfl=40` characters; no default; input required; Name of file with reaction mechanism,
- `outfile`: String of maximum `nfl=40` characters; no default; input required; Name of output file,
- `fam`: Array of maximum `mfam=30` strings, each representing a chemical compound with maximum string length of `nchr=15`; no default; input required.
- `fac`: Array of maximum `mfam=30` real numbers, representing weighting factors; no default; input required,
- `cfam`: String for the family name with maximum string length of `nchr=15` characters; no default; input required,
- `mecca`: Integer for the version number of MECCA (1 or 2).

References

- Jöckel, P., A. Kerkweg, A. Pozzer, R. Sander, H. Tost, H. Riede, A. Baumgaertner, S. Gromov, and B. Kern 2010. Development cycle 2 of the modular earth submodel system (messy2). *Geoscientific Model Development*, 3(2):717–752.
- Jöckel, P., H. Tost, A. Pozzer, M. Kunze, O. Kirner, C. A. M. Brenninkmeijer, S. Brinkop, D. S. Cai, C. Dyroff, J. Eckstein, F. Frank, H. Garny, K.-D. Gottschaldt, P. Graf, V. Grewe, A. Kerkweg, B. Kern, S. Matthes, M. Mertens, S. Meul, M. Neumaier, M. Nützel, S. Oberländer-Hayn, R. Ruhnke, T. Runde, R. Sander, D. Scharffe, and A. Zahn 2016. Earth System Chemistry Integrated Modelling (ESCiMo) with the Modular Earth Submodel System (MESSy, version 2.51). *Geoscientific Model Development*, 9:1153–1200.

Sander, R., A. Baumgaertner, S. Gromov, H. Harder, P. Jöckel, A. Kerckweg, D. Kubistin, E. Regelin, H. Riede, A. Sandu, D. Taraborrelli, H. Tost, and Z.-Q. Xie
2011. The atmospheric chemistry box model caaba/mecca-3.0. *Geoscientific Model Development*, 4(2):373–380.