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Contribution of emissions to concentrations: the TAGGING 1.0 submodel based on the Modular Earth Submodel System (MESSy 2.52)

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Contents

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 O_3 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.

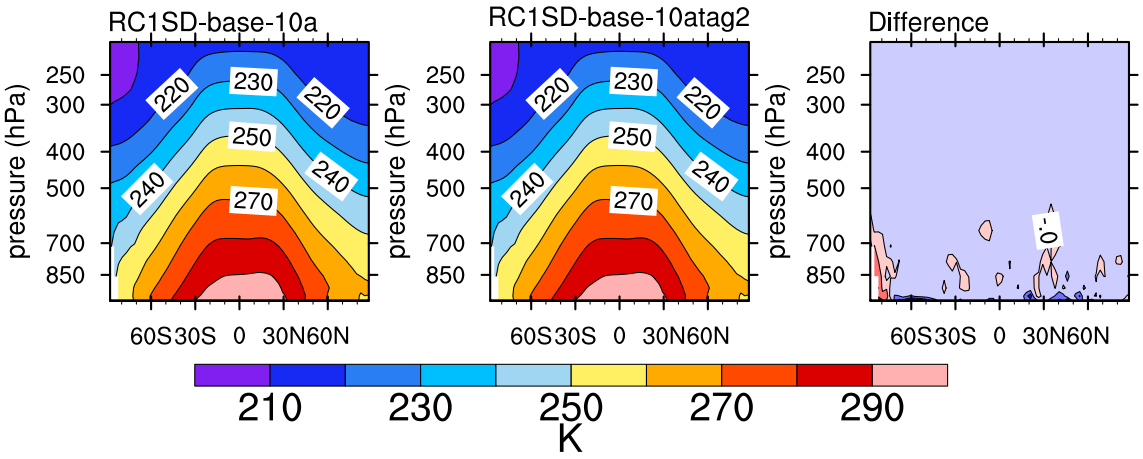

Figure 1: Zonally averaged annual mean temperature (in K) for the time period 2005 to 2010. The left plot shows the value for the RC1SD-base10a, the middle plot the value for the simulation RC1SD-base10a_tag and the right plot the absolute difference between the two fields. The colour bar indicates only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

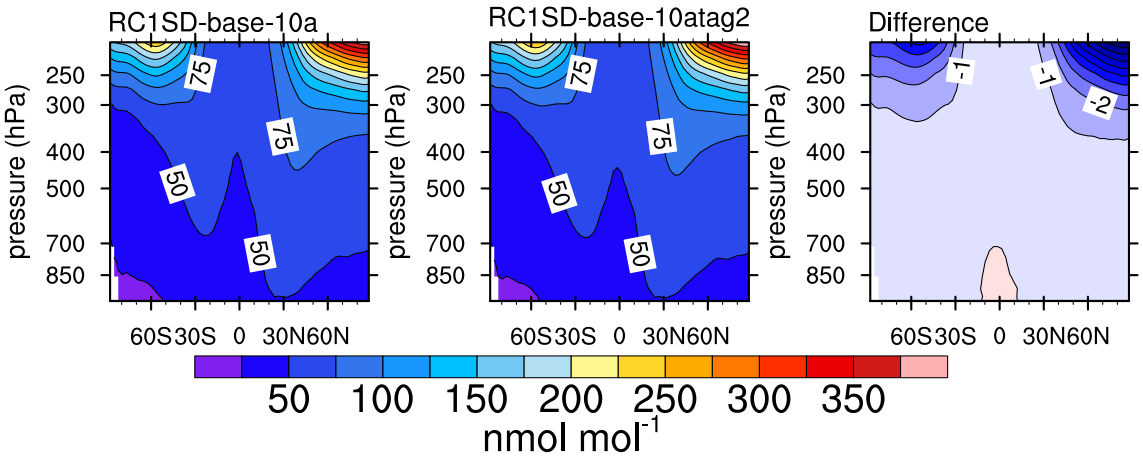

Figure 2: As Fig. 1 but for O_3 (in nmol/mol).

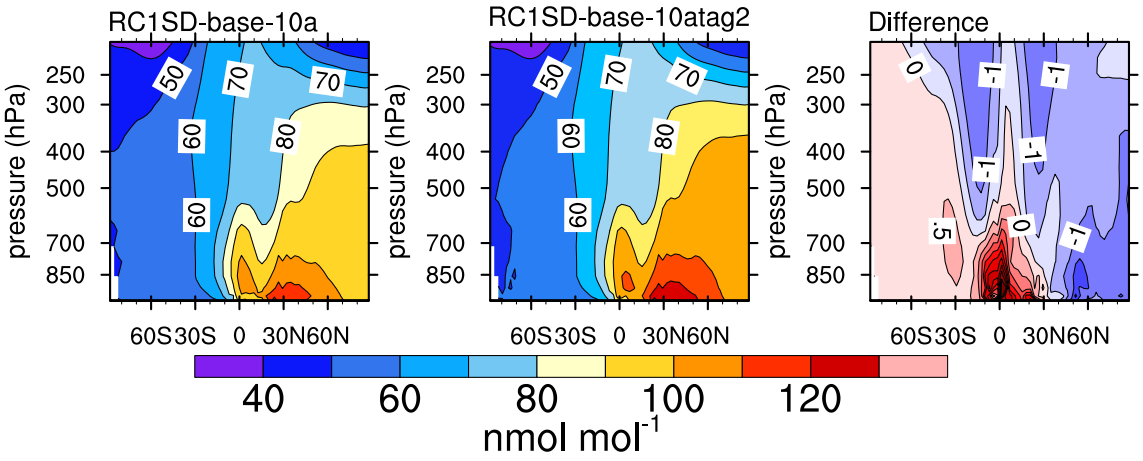

Figure 3: As Fig. 1 but for CO (in nmol/mol).

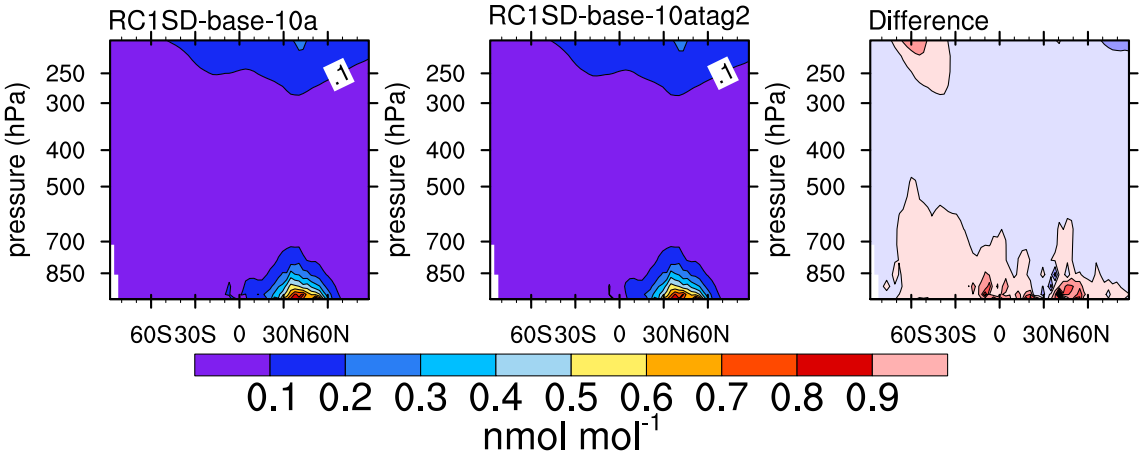

Figure 4: As Fig. 1 but for NO_x (in nmol/mol).

Table 1: Overview on the families NO_y, NMHC, and O_3.

NO_y		NMHC		ODD	
weight: 1					
N	NO	CH_3OH	CH_3O_2	O_3	$O(^3P)$
NO_2	NO_3	CH_3OOH	HCHO	$O(^1D)$	ClO
HONO	HNO_3	HCOOH		HOCl	OClO
HNO_4	NACA			NO_2	HNO_3
MPAN	$IC_3H_7NO_3$			HNO_4	PAN
$LC_4H_9NO_3$	ISON			NACA	MPAN
$ClNO_3$	$BrNO_3$			$IC_3H_7NO_3$	$LC_4H_9NO_3$
				ISON	BrO
				ClO	
weight: 2					
N_2O_5		C_2H_6	C_2H_4	Cl_2O_2	NO_3
		$C_2H_5O_2$	C_2H_5OOH	$ClONO_2$	$BrONO_2$
		CH_3CHO	CH_3CO_2H		
		CH_3CO_3	CH_3CO_3H		
		NACA			
weight: 3					
		C_3H_8	C_3H_6	N_2O_5	
		$IC_3H_7O_2$	IC_3H_7OOH		
		$LHOC_3H_6O_2$	$LHOC_3H_6OOH$		
		CH_3COCH_3	$CH_3COCH_2O_2$		
		HYPERACET	ACETOL		
		MYGLYOX	MPAN		
		$IC_3H_7NO_3$			
weight: 4					
		NC_4H_10	$LC_4H_9O_2$		
		LC_4H_9OOH	MVK		
		MVKO2	MVKOOH		
		MEK	LMEKO2		
		LMEKOOH	BIACET		
		$LC_4H_9NO_3$			
weight: 5					
		C_5H_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 O_3, PAN, CO, OH, HO_2, 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.

Submodel Interface Layer `messy_tagging_si.f90`	*Base Model Core Layer* `messy_tagging.f90`

`tagging_initialize`
Calls subroutines to read `CTRL` and `CPL` namelists
`tagging_read_nml_cpl`
Reads coupling relevant parameters
	`tagging_read_nml_ctrl`
	Reads core relevant parameters

`tagging_new_tracer` Definition of TAGGING tracers	
`tagging_init_memory` Allocation of fields and generation of TAGGING channel objects	
`tagging_init_coupling` Initialise coupling, makes information available from other submodels	

`tagging_init_tracer`
Initialisation of TAGGING tracers, e.g. from restart files or using
`tagging_init_tracer_online`
Online initialisation of tracers in the case of simulation from scratch.	

`tagging_local_start` Store X0 values for chemical fields after transport	
`tagging_vdiff` Compares pre- and after vdiff tendencies of tracers to account for on-line emissions of tracers	

`tagging_physc`
First calculate X1 values, then calculate chemical changes
	`tagging_tendencies`
	Adapt Production and Loss terms to the chosen tagging integration scheme
	`tagging_get_HOx_tendencies`
	Solves equation to get HOx tendencies
	`tagging_get_tendencies`
	Re-Calculate the production and loss terms of the C-compounds based on MECCA output
	`tagging_chemistry`
	Calculate impact of emissions on short-lived species

`tagging_free_memory` Release memory	

3.3 The subroutine `tagging_tendencies`

`ELEMENTAL SUBROUTINE tagging_tendencies`

name	type	intent	description
mandatory arguments:			
General information			
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
X1	`REAL(DP)`	`IN`	species at timestep X1 [mol/mol]
X2	`REAL(DP)`	`IN`	species at timestep X2 [mol/mol]
P	`REAL(DP)`	`IN`	production rate of species [mol/mol/s]
D	`REAL(DP)`	`IN`	loss rate of species [mol/mol/s]
alpha	`REAL(DP)`	`OUT`	correction factor >= 0
beta	`REAL(DP)`	`OUT`	correction factor >= 0

3.4 The subroutine `tagging_HOx_tendencies`

`ELEMENTAL SUBROUTINE tagging_HOx_tendencies`			
name	type	intent	description
mandatory arguments:			
General information			
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:			
General information			
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:			
General information			
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 o3prodro2 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 coresponding 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", "OClO",
"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

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