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Two new submodels for the Modular Earth Submodel System (MESSy): New Aerosol Nucleation (NAN) and small ions (IONS) version 1.0

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Contents

1 IONS

1.1 IONS namelist

The namelist file of the submodel IONS consists of the Fortran namelists CTRL and CPL. The content off each namelist is given in the beginning of each subsection. The combined namelist file is obtained by concatenating the individual namelists.

1.1.1 CTRL

Variables set in the namelist CTRL control the overall behaviour of the submodel.

```
&CTRL
gcr_method = 2
lqradon = .TRUE.
laero=.true.
/
```

- the integer variable `gcr_method` defines the method used for ion pair production rate due to GCR currently possible values are 0 for no GCR ionisation and 2 for GCR ionisation according to [Usoskin et al., 2010].
- Radon decay is included in the calculation of ion production, if `lqradon` is set to `TRUE`.
- `laero` determines if ion aerosol coupling should be included in the calculation of steady state ion concentrations.

1.1.2 CPL

The `CPL` namelist sets variables needed for coupling to other submodels.

```
&CPL
phi  = 'import_ts','phi'
igrf = 'import_ts','igrf'
lssion =.true.
ltotalipr =.true.
cpl_aero_r = 'gmxe_gp', 'wetradius'
cpl_aerocon = 'gmxe_gp', 'anumber'
/
```

`igrf` and `phi` define which submodel provides the time series for the geomagnetic field and the GCR modulation. These variables are of MESSY's `t_chaobj_cpl` derived data type and contain the string variable `cha`, which defines the name of the submodel that imports the time series, and the variable `obj`, the name of the channel object. In the example namelist file the importing channel is `import_ts`.

Ion aerosol interaction is defined by coupling IONS to variables from the aerosol models. The ion aerosol attachment coefficient can be calculated from aerosol particle concentration and radius. Alternatively, the condensation sink of a vapour, e.g. sulphuric acid, can be used as the ion-aerosol attachment coefficient by defining the coupling type.

- If the aerosol submodel provides a condensation sink, number of lost ions s^{-1}, as a channel object it can be retrieved with `cpl_aero_cs`
- the radius of the the aerosol particles, in m, can be used by coupling to the radius via `cpl_aero_r`
- and `cpl_aerocon` for the aerosol particle number concentration in cm^{-3}.

1.2 Additions in import.nml

The variable name and path to time series and look up tables have to be included in the namelist file of the import submodel. For the time series this is in the namelist `CTRL_TS`:

```
&CTRL_TS
...
TS(4) = 'phi',  '$INPUTDIR_MESSY/misc/MPIC_monthly1.0_hist_X_Phi_195101-201612.txt'
TS(5) = 'igrf', '$INPUTDIR_MESSY/misc/MPIC_1.0_hist_X_GUFMIGRF12_1590_2014.txt'
..
/
```

The look up table for the GCR induced ionisation has to be included in the namelist `CTRL_LT`:

```
LT(1) = 'CRII', '$INPUTDIR_MESSY/LT_MPIC_1.0_CRII.nc', 'CRII'
```

1.3 IONS channel objects

The IONS submodel provides output to other submodels as channel objects. Tracers or tracer tendencies are not changed in this submodel. The following objects are all defined as `GP_3D_MID` objects.

- `total_ipr` is the total ion pair production rate, the sum of ion pair production by GCR and Radon decay. Values are in cm^{-3} s^{-1}.
- `small_ions_neg` and `small_ions_pos` are the concentration of small positive and negative ions assuming a steady state. Values are given in cm^{-3}.
- `krec` is the recombination rate constant in cm^6 s^{-1}.
- `radon_ipr` is the ion pair production rate from Radon decay in cm^{-3} s^{-1}. This channel object is only created by IONS if `lqradon` is `.TRUE.` and `cpl_ipr_Rn%cha` was not set in the CPL namelist.

- `gcr_ipr` is the ion pair production rate from galactic cosmic rays in cm^{-3} s^{-1}. This channel object is only created by IONS if `lgcr` is `.TRUE.` and `cpl_ipr_gcr%cha` was not set in the CPL namelist.

- `aero_cs` is created by IONS if `laero` is set to `.TRUE.` and `cpl_aero_cs%cha` is set to an empty string or not initialised. `aero_cs` is the loss rate of ions onto aerosol particles in cm^{-3} s^{-1}.

2 NAN

2.1 NAN namelist

2.1.1 CTRL

```
&CTRL
lselnuc(1) = .FALSE.
lselnuc(2) = .FALSE.
lselnuc(3) = .FALSE.
lselnuc(4) = .TRUE.
lselnuc(5) = .TRUE.
lselnuc(6) = .TRUE.
lselnuc(7) = .TRUE.
lselnuc(8) = .TRUE.
lselnuc(9) = .TRUE.
lselnuc(10) = .TRUE.
nnucspec=4
nuclmethod='multi'
/
```

The set of nucleation parameterisation can be chosen via `lselnuc`. This variable is a vector of logical values, the index indicates the nucleation parameterisation, see table 1. `lselnuc(3)` is not included in table 1 as it was originally used for the parameterisation given in [Merikanto et al., 2007]. However, this parameterisation required mixing ratios instead of vapour concentration. Due to more recent parameterisations from other sources the parameterisation is not fully implemented. Additionally the number of nucleating vapour species must be defined by `nnucspec`. A string variable indicating the algorithm used must be provided by `nuclmethod`. For multi-component nucleation this should be set to `'multi'`. If GMXe is used the [Vehkamäki et al., 2002] parameterisation can be used by setting `nuclmethod` to '`vehk_gmxe`'.

Table 1: Summary of `lselnuc` variables in the `CTRL` namelist, default value for all is `.FALSE.`.

Variable	Parameterisation	involved species
`lselnuc(1)`	[Vehkamäki et al., 2002]	H_2SO_4
`lselnuc(2)`	[Kulmala et al., 1998]	H_2SO_4
`lselnuc(4)`	[Dunne et al., 2016]	H_2SO_4
`lselnuc(5)`	[Dunne et al., 2016]	H_2SO_4, n^-
`lselnuc(6)`	[Dunne et al., 2016]	H_2SO_4, NH_3
`lselnuc(7)`	[Dunne et al., 2016]	H_2SO_4, NH_3, n^-
`lselnuc(8)`	[Riccobono et al., 2014]	H_2SO_4, Organic
`lselnuc(9)`	[Kirkby et al., 2016]	H_2SO_4, Organic
`lselnuc(10)`	[Kirkby et al., 2016]	H_2SO_4, Organic, n^-, n^+
`lselnuc(11)`	[Almeida et al., 2013]	H_2SO_4, Amines

2.1.2 NUC

```
&NUC
sulphuric_acid="H2SO4"
ammonia="NH3"
amines="LAMINE"
HOMOH="HOMOH"
HOMO3="HOMO3"
/
```

The only variables to set in the namelist `NUC` are the names of the nucleating vapours. This is important if the name of the species differs from the default name assumed in NAN. The variable names and default names are given above.

2.1.3 PARAM

```
&PARAM
dunne_pbn=3.95451
dunne_ubn=9.702973
dunne_vbn=12.62259
dunne_wbn=-0.007066146
dunne_ptn=2.891024
dunne_utn=182.4495
dunne_vtn=1.203451
dunne_wtn=-4.188065
dunne_pAn=8.00
dunne_an=1.6d-6
dunne_pbi=3.37
dunne_ubi=-11.48166
```

```
dunne_vbi=25.49469
dunne_wbi=0.1810722
dunne_pti=3.14
dunne_uti=-23.8002
dunne_vti=37.03029
dunne_wti=0.227413
dunne_pAi=3.07
dunne_ai=0.00485

kirkby_a = 0.04001, 1.848, 0.001366, 1.566, 0.1863

ricco_k=5.45d-19 !3.27e-21 ! Riccobono et al 2014

frhc1=1.5
frhc2=0.045
BtdOrg = 0.0
l_Dunne_RH =.FALSE.
l_org_Tdep=.FALSE.
/
```

The namelist `PARAM` gives a large set of tuning parameters for the parameterisations. All parameters can be changed here without recompiling the model. A full list of parameters is given in table 2 together with the parameter symbol used in the main manuscript and the default value. The logical variables `l_org_Tdep` and `l_Dunne_RH` are not included in the tables since they provide simple switches for RH dependency of inorganic nucleation and temperature dependency for organic nucleation.

Table 2: Summary of variables in the namelist `PARAM`, default value and symbol used in the main manuscript is also given.

variable	default value	symbol
`dunne_pbn`	3.95451	$p_{b,n}$
`dunne_ubn`	9.702973	$u_{b,n}$
`dunne_vbn`	12.62259	$v_{b,n}$
`dunne_wbn`	-0.007066146	$w_{b,n}$
`dunne_ptn`	2.891024	$p_{t,n}$
`dunne_utn`	182.4495	$u_{t,n}$
`dunne_vtn`	1.203451	$v_{t,n}$
`dunne_wtn`	-4.188065	$w_{t,n}$
`dunne_pAn`	8.00	$p_{a,n}$
`dunne_an`	1.6d-6	a_n
`dunne_pbi`	3.37	$p_{b,i}$
`dunne_ubi`	-11.48166	$u_{b,i}$
`dunne_vbi`	25.49469	$v_{b,i}$
`dunne_wbi`	0.1810722	$w_{b,i}$
`dunne_pti`	3.14	$p_{t,i}$
`dunne_uti`	-23.8002	$u_{t,i}$
`dunne_vti`	37.03029	$v_{t,i}$
`dunne_wti`	0.227413	$w_{t,i}$
`dunne_pAi`	3.07	$p_{a,i}$
`dunne_ai`	0.00485	a_i
`kirkby_a(1)`	0.04001	a_1
`kirkby_a(2)`	1.848	a_2
`kirkby_a(3)`	0.001366	a_3
`kirkby_a(4)`	1.566	a_4
`kirkby_a(5)`	0.1863	a_5
`ricco_k`	5.45d-19	k_{Ric}
`frhc1`	1.5	c_1
`frhc2`	0.045	c_2
`BtdOrg`	0.0	B

2.1.4 CPL

```
&CPL
cpl_ipr%cha='ions'
cpl_ipr%obj='total_ipr'
cpl_krec%cha='ions'
cpl_krec%obj='krec'
cpl_klion%cha='ions'
cpl_klion%obj='aero_cs'
lnucten=.TRUE.  ! add new particles as tendencies, default
```

```
driver_call='radiation'
b4gmxe = .FALSE.
/
```

CPL controls the coupling of NAN to other submodels. The new parameterisations rely heavily on ion aerosol interaction, therefore several variables of the t_chaobj_cpl type are used here for coupling to the IONS submodel.

- cpl_ipr defines the channel and channel object for the ion pair production rate in cm^{-3} s^{-1}.
- cpl_klion is the ion-ion recombination in cm^6 s^{-1}.
- cpl_coags is the ion aerosol loss in cm^3 s^{-1}.
- aerosolmodel is a string variable and allows to set the channel name of the aerosol submodel, default is "GMXE".

Additionally to coupling to other submodels this namelist allows to control where in the Base Model Layer NAN is called.

- driver_call a string variable that can take the values "radiation" or "physc". Depending in whether the nucleation should be called in the radiation or general physics part of the base model. The default value is "physc"
- b4gmxe a logical value of TRUE indicates that NAN is called before GMXe. If set to FALSE NAN will be called after GMXe. This option makes only sense if driver_call is used to ensure that GMXe and NAN are called in the same basemodel subroutine.

Interaction between NAN and other aerosol models is further refined by the following variables

- lnucten a logical variable that defaults to .TRUE.. A true value results in NAN calculating nucleation mode particle tendencies, otherwise the tendency is not updated by NAN.
- lnucmode a logical variable, if .TRUE. NAN calculates the formation rate of particles in the nucleation mode, else the produced particles are grown to a size given by cpl_d2
- cpl_d2 is a t_chaobj_cpl type variable that is set to the aerosol models lower mode diameters.

2.2 Channel Objects

The NAN submodel provides several channel objects that can be used by other submodels.

- The number of freshly produced particles per unit volume is `panew` as number of particles cm^{-3}.
- `nucrate` is the total formation rate of new particles in particles cm^{-3} s^{-1}. Individual formation rates for each nucleation channel are also provided. Their channel object name is the same as the nucleation channel name within NAN.
- The use of `panew` or `nucrate` provides an alternative to updating the aerosol particle tracer tendency. If the `lnucten` is set to `.FALSE.` and the coupled aerosol model uses `panew` or `nucrate` to calculate the particle concentration.

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