

GMXe – Users Manual

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1 Introduction

GMXe is a global aerosol microphysics and thermodynamics module, implemented within the EMAC (ECHAM5/MESSy Atmospheric Chemistry) GCM (Joeckel *et al.* 2005). The model consists of an aerosol model (based on an extended version of the M7 model, Vignati *et al.* 2004) coupled to a choice of gas / aerosol partitioning models: EQSAM3 (Metzger and Lelieveld 2007) or ISORROPA-II (Fountoukis and Nenes, 2007). Both the microphysics and the partitioning elements are contained within a single EMAC submodel, called GMXe.

The model is designed to be highly flexible with regard to the number and type of species simulated and the modelling assumptions used. However, along with this flexibility comes a degree of complexity, and for useful simulations it is vital to set-up the model correctly. This users' manual is designed as a supplement to the model description paper, and its aim is to help the user set-up and run the model within EMAC.

The details in this manual refer to version 1.0 of GMXe, implemented within the EMAC v1.8, as described in Pringle *et al.* (*submitted to Geoscientific Mode Development Discussions*). The manual describes some of the GMXe code and explains a typical set-up of the namelist file. An example set-up of the file that controls model emissions is then given.

Running GMXe in EMAC – Global simulations

The GMXe module is turned on / off in the same manner as other EMAC submodels: simply set `USE_GMXe=TRUE` in the `xmessy` file. When running GMXe, it is important to switch off other available aerosol models (M7 and MADE) in `xmessy`. The `xmessy` file also has the option to run an older version of EQSAM as a separate submodel, however for GMXe runs the `USE_EQSAM` switch should be set to `FALSE` as EQSAM3 is integrated within GMXe model.

Interaction with other submodels

The aerosol distribution simulated can be used by two other submodels in EMAC: SCAV and HETCHEM. The SCAV submodel (Tost *et al.* 2006) treats the wet deposition of aerosols and gases. SCAV is flexible and can be coupled to any of the aerosol models available in EMAC. To ensure that SCAV is correctly coupled to GMXe, set `aermod`, `sigma` and `aerrad` to 'gmXe' in the name list `scav.nml`.

The HETCHEM submodel treats the heterogeneous chemistry on the surface of the aerosols. The namelist `hetchem.nml` controls which aerosol distribution is used for the heterogeneous chemistry. To couple GMXe to HETCHEM set `L_H2SO4_prescribed = .F.` (so the climatological aerosol distribution is *not* used) and set: `sigma_nml`, `rdrya_nml`, `rweta_nml`, `dweta_nml`, `anumb_nml` all = 'gmXe'. Alternatively, an aerosol climatology can be used to calculate heterogeneous chemistry, set `L_H2SO4_prescribed = .T.`, (recommended, as used in standard run).

Notation

The microphysics of GMXe are fundamentally the same as that of the M7 (Vignati *et al.* 2004), however, one thing to note when referring to the work of Vignati *et al.* (2004) is that where the M7 documentation refers to "soluble" and "insoluble" modes in GMXe use the terms "hydrophobic"

and “hydrophilic” modes. This is just a matter of terminology and does not represent difference in the two models.

Overview

The GMXe code consists of 4 main parts:

- e5 level source code: *messy/e5/messy_gmXe_e5.f90*
- Namelist files: *messy/nml.B/gmXe.nml*
- Parameter file: *messy/src/messy_gmXe_parameters.inc*
- Source code: *messy/src/messy_gmXe.f90*

The next sections of this document will introduce each of these parts and explain the main options available.

2 e5 level code

The purpose of the “e5 code” is to pass information to and from GMXe to the rest of the EMAC model, i.e. it deals with the coupling of the GMXe aerosol model to EMAC.

Four main processes are carried out in this level:

- The aerosol emissions streams provided by the ONLEM and OFFLEM submodels are used to update the aerosol tracer tendencies (Kerkweg et al 2006), including the division of the bulk species into different aerosol species (See Section 4).
- The subroutine *gmXe_main* is called. It is this subroutine which contains the GMXe source code (stored in the file *messy_gmXe.f90*).
- After the call to *gmXe_main*, the tracer tendencies are updated, thus the aerosol gas / distribution in EMAC is updated to account for the changes calculated by GMXe.
- Code is called to check that the GMXe model is mass conserving (if mass violation errors occur this will be written to the log file in the WORKDIR).

3 Namelist file

Much of the complexity of the GMXe model is controlled via the *gmXe.nml* namelist file, it is here that individual microphysical processes can be turned on and off, and many settings can be controlled. The following section lists the switches available and briefly summarises the purpose of each and gives a recommended setting (i.e. the setting used in the *Geoscientific Mode Development Discussions* paper). An example namelist setting is given in Appendix 1.

Switches controlling the interaction with EMAC

LGMXe: *Aerosol composition scheme GMXe (interface).* If LGMXe=F then *gmXe_main* (and hence GMXe) is not called, only the e5 level code is called. Recommended: LGMXe = .T.

LOUTPUT: *Write GMXe stream to diagnose output.* Switch controls whether a netCDF file, containing details of the aerosol number / size distribution is written to the working directory. Recommended: LOUTPUT = T.

LMASS_DIAG: *Mass balance check in gmXe_physc.* If TRUE the total gas + aerosol mass is summed before and after call to *gmXe_main* (e5 level). Error messages are printed if the total

mass after the call to GMXe is not equal to that before (i.e. if the GMXe model setup is not mass conserving). Recommended: LMASS_DIAG = T.

LSTRAT: *Exclude stratosphere (requires TROPOP stream).* If LSTRAT = T model does not update tracer tendencies for gridboxes in the stratosphere (e5 level). Recommended: LSTRAT = F.

LPSC: *Exclude PSC region (requires PSC stream).* If LPSC = T, then the model does not update tracer tendencies in any regions where PSC formation is possible (e5 level). Recommended: LPSC = F.

Switches controlling the aerosol microphysics

LNUCL: *Calculate nucleation of aerosol particles.* If LNUCL = T; the model calculates new particle formation of sulfate particles following either a standard nucleation scheme (Kulmala or Vehkamaeki) or a testing one. The choice of nucleation scheme is determined by the NNUCL switch (see below). Recommended: LNUCL = T.

LCOND: *Calculate the amount of condensable species due to kinetic limitations.* If LCOND=T, the model limits the amount of gas phase material available for condensation (pgasi) by considering the kinetic limitations to condensation. pgasi is calculated in gmXe_dgas. A note of caution: LCOND does **not** switch on / off condensation of gas to aerosol; it switches on / off consideration of the kinetic limits to condensation. Recommended LCOND = T.

LCOAG: *Reshape the size distribution due to particle coagulation.* LCOAG switches on / off the coagulation of aerosol particles (controls call to gmXe_coaset and the parameters passed into gmXe_delcoa). Recommended: LCOAG = T.

LSIZE: *Reshape the size distribution due to hygroscopic growth.* LSIZE=T is an experimental setup in which the re-distribution of aerosol between modes (due to growth by condensation or coagulation) is done based on the aerosol wet radius. In this setup, the call to gmXe_dconc is switched off to avoid double counting. If LSIZE = F redistribution of the aerosol between the modes is done in gmXe_dconc, based on the dry radius. Recommended: LSIZE = F (redistribution will then be done in the same way as the M7, this is more consistent as the GMXe / M7 mode boundaries are based on the dry aerosol size).

LCOAT: *Calculate coating/ageing of primary particles.* LCOAT controls the transfer of particles from the insoluble to the soluble modes, if sufficient hydrophilic material is condensed on the hydrophobic aerosol, the hydrophilic material (and a fraction of the hydrophobic material) are transferred to the hydrophilic modes. Done within gmXe_thermo (the interface that calls the partitioning schemes), thus NEQM must be > -1 for it to work. Recommended: LCOAT = T.

LAH2O: *Calculate aerosol water concentration limited by specific humidity (otherwise equilibrium is assumed).* If LAH2O = T the model limits the amount of water vapour available for uptake to the aerosol by the specific humidity. If LAH2O = F then the available water vapour is unlimited and the aerosol can take up as much water as is needed to achieve equilibrium for all its components. Recommended: LAH2O = T.

LSHUM: *Update specific humidity (ECHAM5).* If LSHUM=T then and change in specific humidity calculated in GMXe, due e.g. to the uptake of water on aerosols, is allowed to feedback to the ECHAM5 specific humidity. Recommended: LSHUM = F.

Switches controlling aerosol cloud coupling

The following section of the namelist file deals with aerosol-cloud coupling, at present this should always be switched off (LACC = F) as this section of the code is experimental. All switches associated with ACC should also be set to false (LCLC, LADYN, LCLWC, LCIWC, LCDNC and LICNC).

Switches controlling the aerosol setup

LGAS: Update gas phase chemistry, and **LAEROSOL:** Update aerosol phase chemistry. Setting LGAS or LAEROSOL to F means that any changes to the aerosol / gas concentrations calculated within GMXe are not used to update the gas / aerosol tracers on the e5 level. In effect this means that GMXe will calculate a change in tracers but any change will be disregarded and GMXe will have no effect (i.e. the change in tracer tendency will be set to zero in e5 level). Thus the model will not update gas (or aerosol) tracer concentrations. Recommended LGAS = LAEROSOL = T.

LNUMBER: Calculate aerosol numbers from aerosol mass. GMXe can either transport aerosol numbers as a prognostic tracer, or it can simply calculate number from aerosol mass. Setting LNUMBER=F means that number is carried as a tracer (same as M7). Recommended LNUMBER = F.

LWETRAD, LDRYRAD, LDRYDENS: .T. = Calculate aerosol wet radius / dry radius / dry density from EQSAM3 / ISORROPIA. F= from bulk. If LWETRAD, LDRYRAD or LDRYDENS= T then wet / dry radius and aerosol density calculated in ISORROPIA / EQSAM3 are used. For this to be effective NEQM must be > 0. If = F, then the properties calculated for bulk species (in gmXe_averageproperties) are used. Recommended: LWETRAD = LDRYRAD = LDRYDENS = T.

Calculate aerosol composition and hygroscopic growth for selected modes:

Default values:

NLOWERMODE = 1 ! Lowest mode (min. mode number = 1; nucleation mode, soluble)

NUPPERMODE = 7 ! Upper mode (max. mode number = 7; coarse mode, insoluble)

GMXe has the option to choose to apply gas / aerosol partitioning to only a sub-section of the aerosol modes. In the standard model setup (above) the thermodynamics is calculated for all of the modes (modes 1-7). At the moment, the transfer of mass from hydrophobic to hydrophilic modes is done in the interface routine (gmXe_thermo), thus for this to occur, the mode must be within the range of NUPPERMODE to NLOWER mode. Recommended: NLOWERMODE = 1, NUPPERMODE =7.

NEQM: Choice of thermodynamic module: -1, 0 = None (bulk hyg growth only), 1= EQSAM3h, 2= ISORROPIA2, [-1 = no partitioning interface (gmXe_thermo), only gmXe core]. The NEQM switch controls whether the EQSAM3 / ISORROPIA gas / aerosol partitioning models are used. Four settings are possible:

- NEQM = -1 turns off all calls to the partitioning models and the model is run without thermodynamics (similar to the M7).
- NEQM = 0 is an intermediate switch where the interface to the partitioning is called, but the partitioning model itself is not (NEQM=0 is for testing only).
- NEQM = 1 with this EQSAM3 is called and the GMXe model is run with gas / aerosol partitioning as calculated by EQSAM3.
- NEQM = 2 with this ISORROPIA is called and the GMXe model is run with gas / aerosol partitioning as calculated by ISORROPIA

NNUCL: Choice of nucleation scheme. 0 = test, 1 = Vehkamaeki (2002), 2 = Kulmala (1998). NNUCL controls the choice of nucleation scheme used to calculate formation of sulfate particles.

This is only relevant if LNUCL = T (above). NNUCL = 0 is still under development. Scheme 1 (Vehkamaeki) is recommended as its valid over a greater temperature range than Kulmala (1998).

Switches that control the settings in EQSAM3.

The following switches concern the setup of the EQSAM3 model, and thus are only relevant if NEQM=1.

LSKIP: *Calculations only for non-zero compounds / solutes (global modelling).* LSKIP is used within eqsam3_v01h to say that if the mass of the sum of all aerosol species in a particular mode is very small then calculation of the partitioning is skipped. Recommended: LSKIP = T.

LDRY: *Force aerosol particles to be dry (no aerosol water).* Setting LDRY = T stops the aerosols taking up water; the aerosols are assumed to be dry under all conditions, this is for sensitivity studies only. Recommended: LDRY = F.

LSOLIDS: *Inclusion of solid aerosol particles (if false, only metastable).* If LSOLIDS = T then EQSAM3 permits solids to form within the aerosol when the conditions such that solids would form. One can force the aerosol particle to remain liquid under all conditions by setting LSOILDS = F. Recommended: LSOLIDS=T.

LRHDMIX: *Use RHD and RHcr of mixed solutions (.F. RHDs/RHcr of single solutes are used).* If LPREORD = F (see below) the model calculates a single solute precipitation order. If LRHDMIX=F then this precipitation order is based on single solutes, if LRHDMIX=T then the efflorescence and deliquescence RHs of mixed solutions are used. (Note RHD = Deliquescence RH and RHcr is the RH of Crystallisation). Recommended LPREORD = T (therefore no recommendations for this switch)

LHYSTER: *Inclusion of hysteresis effect (includes solids/metastable).* If LHYSTER is set to true then the aerosol water content is used to define aerosol as “wet” or “dry”, in order to decide which branch of the hysteresis curve the particle is on, and thus which critical RH should be used. If LHYSTER = F, aerosol are all assumed to be on the upper (wet) branch. Recommended: LHYSTER = T.

Switches not set within the namelist file

There are also switches that are set within messy_gmXe.f90, rather than the name list file, these switches concern detail in the set-up of GMXe and are not in the namelist file as they are unlikely to be changed frequently. Of course, when a switch in the messy_gmXe.f90 code is changed, the model must be re-compiled for the change to take effect. The two most important switches are explained below, the others should not be changed from their default values.

lpreord: *Use predefined precipitation (reaction) order (.FALSE. = T-dependent RHDs/RHcr = recommended).* EQSAM3 has the option to calculate a single solute precipitation order interactively, taking the deliquescence and efflorescence RH of the simulated species and the temperature into account (if LPREORD = F). If this is not desired, a standard pre-defined precipitation order can be used (the Hofmeister Series, LPREORD = T). See Metzger and Lelieveld (2007) for details. Recommended: LPREORD = T.

luptake: *Uptake of gases on wet and or acid aerosol particles (under development).* If luptake = TRUE, then in EQSAM3, after the calculation of the expulsion of non-paired species, the pure acid species are then potentially allowed to dissolve in the aerosol water (recommended LUPTAKE = FALSE).

The ISORROPIA-II model

The source code for the ISORROPIA-II model is stored in the directory `libsrc/isorroopia`, a detailed description of the model can be found at: <http://nenes.eas.gatech.edu/ISORROPIA/> which contains both the original publications and a detailed users' manual (Fountoukis and Nenes 2007; Nenes et al. 1998).

4 Parameter File

The flexible nature of GMXe allows one to simulate aerosol distributions with a wide range of different complexities – the model can be run with just a couple of “bulk” aerosol species or it can be run in much more complex setups, where it treats the major species within each bulk aerosol type (i.e. the main cations / anions in the aerosol system).

The number and type of species simulated is controlled in the `messy_gmXe_parameters.inc` file. The parameter file is divided in to three sections:

- *Section (A)*: Outlines the basic aerosol mode parameters e.g. the mode boundaries and the assumed standard deviation of each mode.
- *Section (B)*: Controls which species are permitted to exist in each mode
- *Section (C)*: Controls the division of the bulk emission fluxes between the different species.

Section A: Standard mode parameters

The model simulates `nmod` aerosol modes (`nmod = 7`); mode 0 is the gas phase then modes 1:`nmod` are the soluble and then the insoluble modes. Normally there are 4 soluble and 3 insoluble modes (in order): NS = nucleation soluble, KS = Aitken soluble, AS = accumulation soluble, CS = coarse soluble, KI = Aitken insoluble, AI = accumulation insoluble and CI = coarse insoluble.

The dry radius mode boundaries (`crdiv`) and the assumed standard deviation of the aerosol modes (`sigma`) are also set in this section. The array `caccgas` sets the assumed mass accommodation coefficient of the gas phase species.

Section B: “Inclusion / exclusion of individual ions”

Section B of the parameter file allows the user to switch particular species on or off in each of the different modes. The species are switched on / off using a simple logical switch. The species are grouped into 6 different categories: acids, cations, anions, solutes, bulk and one salt.

Each species has an “L_NAME” array with 8 dimension (gas phase and then 7 aerosol modes; the *NAME* section dictates the species' name). For example, `L_H2SO4` switches on / off H2SO4 in the gas and aerosol phase. If one wanted to simulate H2SO4 in the gas phase and the soluble nucleation mode only, `L_H2SO4` would be set as follows:

```
! Aerosol mode names      gp      ns      ks      as      cs      ki      ai      ci
LOGICAL, PARAMETER::L_H2SO4 (0:nmod)=(/.TRUE. .,TRUE. .,FALSE.,FALSE.,FALSE.,FALSE.,FALSE.,FALSE./)
```

Care must be taken when setting up the model as not all the `L_NAME` options make physical sense; the user must carefully consider what setup is needed.

Caution: some possible settings of the L_NAME arrays can lead to mass violations, in general this happens if an anion is treated in the aerosol phase without allowing for the corresponding acid. For example, if L_CHLORIDE is switched on in the aerosol phase and EQSAM3 is switched on (NEQM=1) then L_HCL must be permitted in the gas phase. If mass violations occur an error message will be printed in the log file.

Section C: “Enrichment factors for primary emissions”

GMXe has the capability to also simulate cations / anions within the aerosol distribution. However, the aerosol emission fluxes in the model are bulk fluxes, thus the model needs to divide these bulk fluxes into “chemically speciated” fluxes. This division of the bulk aerosol fluxes into speciated emissions is done in Section C of the *messy_gmXe_parameters.inc* file.

GMXe considers the primary emission of 4 bulk species: sea salt (SS), black carbon (BC), organic carbon (OC) and dust (DU). The EMAC model (ONLEM / OFFLEM) provides a flux of each of these bulk species. As these different bulk species are emitted at different sizes, the emission fluxes are given by the emission routines in different size categories (see *messy_gmXe_e5.f90*):

- Sea salt is emitted in the accumulation and coarse soluble modes (AS & CS)
- BC is emitted in the insoluble Aitken mode (KI)
- OC is split between the insoluble and soluble Aitken modes (KS & KI)
- DU is emitted in the coarse insoluble modes (CI)

In Section C of the parameter file, there is a F_XXXX_NAME array for each species and for each of the bulk fluxes (e.g. XXXX = SeaSalt, Organic, BCarbon or Dust and NAME is the species name e.g. CHLORIDE). F_XXXX_NAME represents the mass fraction of the bulk flux (per mode) that is put into a particular species. Again each array has 8 dimensions; gas phase plus the 7 aerosol modes.

The process is perhaps best explained through the use of an example; let’s consider how to speciate the bulk sea salt emission flux into a flux of sodium and chloride with an ionic ratio of 1:1. The sea salt flux is calculated in ONLEM, giving a flux of bulk sea salt aerosol into AS and CS modes. To split the total bulk flux into the individual compounds the F_SeaSalt_CHLORIDE and F_SeaSalt_SODIUM arrays must be given non-zero values. If no other species are to come from the sea salt then all other L_SeaSalt_NAME array entries should be zero.

When choosing the emission factor, care must be taken to consider the relative mass fractions of the species in the setup. In our example we want to split the sea salt flux into a sodium and a chloride flux assuming a 1:1 ratio of Na:Cl ions in the sea salt. The relative mass fractions of the species would then be:

```

! Aerosol modes
REAL(dp), PARAMETER :: F_SeaSalt_SODIUM (0:nmod) = (/0.000,0.000,0.000,0.390,0.390,0.000,0.000,0.000/)
REAL(dp), PARAMETER :: F_SeaSalt_CHLORIDE (0:nmod) = (/0.000,0.000,0.000,0.610,0.610,0.000,0.000,0.000/)
REAL(dp), PARAMETER :: F_SeaSalt_BULK (0:nmod) = (/0.000,0.000,0.000,0.000,0.000,0.000,0.000,0.000/)

```

Mass fraction Na = (molecular weight Na)/(total molecular weight NaCl). Note that the non-zero values are in the AS and CS modes, as it is in these modes that sea salt is emitted.

The F_XXXX_BULK array controls the fraction of the species that goes into the bulk distribution. This is typically the fraction ‘left-over’ after speciation. In the above sea salt example, all the mass was speciated so F_SeaSalt_BULK = 0.0 in all modes. But it is not always desirable to speciate all the aerosol, for example, one may want 10% of the emitted dust mass to be calcium carbonate and the rest to be treated as bulk dust mass. For this set F_Dust_Calcium = 0.035 F_Dust_CO3 = 0.052 and F_Dust_BULK = 0.783 (in the CI mode, as that’s where the mass is emitted).

Note that in the dust example above, the sum of the emitted species adds up to 0.87 (not 1.0), this accounts for the fact that a mass stream of 90% bulk dust and 10% CaCO₃ will have a larger mass than one consisting of 100% bulk dust (as the molecular weight of bulk dust is assumed to be 40g). Care must be taken to ensure that one does not accidentally change the total mass of emitted aerosol. Each bulk species has an assumed molecular weight (as used in ONLEM / OFFLEM): Du = 40, SS = 58.5, BC = 12 and OC = 12).

The F_XXXX_MODE arrays control the mass fraction of the total aerosol emission flux that is used, e.g. if, for a sensitivity study, one wanted to half the sea salt emissions flux (without changing the relative chemical speciation) one could simply set F_SeaSalt_MODE to 0.5 (in the AS and CS modes). Normally F_XXXX_MODE = 1 in the modes where the aerosol is emitted (e.g. KI for BC, KI and KS for OC). The exception is for mineral dust, as is advisable to split the bulk mass of dust emitted between the AI and the CI modes, as emitting only in the CI mode is unrealistic.

Finally, it is also important to consider the ionic balance of the emitted aerosol; it is normal to assume that the cations and anions are emitted in a ratio that results in a neutral aerosol.

Parameter file checking – parameter_script

The *messy_gmXe_parameter.inc* file is rather long, but correct settings here are imperative to the correct setup of the model. As an additional checking facility, a Unix script has been developed to summarise the key components of the parameter file. This script is stored in */messy/mbm/gmXe* and is called "*parameter_script*" (to run type `sh parameter_script`). The script simply prints out all values of the L_NAME and F_NAME arrays that are non-zero; it prints out, per mode, which species are allowed ("turned on") and the chosen emission factor. At present this script works only on Grand (not Blizzard).

5 Source Code – Introduction to indices

The *messy_gmXe.f90* file contains the GMXe source code, this file is the core of the model and contains the subroutines dealing with the aerosol microphysics and thermodynamics. This code does not need changed to run the model in different setups (only for model development work).

For code development it is useful to have an understanding of the index arrays used in the model. The *gmXe_main* code uses a range of lookup tables and multi dimensional arrays in the code, which rely on indices. The indices are set up in the routine *eqsam3_initialize_compounds* and a summary is printed out in the log file as the model runs.

There are two "types" of index; those beginning with the letter "c" are character indexes and give the names of the species. Those beginning with the letter "i" are integer indexes and are the actual integers used by the model. When modifying the code, care must be taken to set up the indices, especially in a loop as the index array required depends on what loop you are looping over. The main indices are:

1) Only species dependent:

- *icomp_tr*: is the unique index for the species type – every species has a unique *icomp_tr* value, which is *independent* of which mode it's in (e.g. 2 for sulphuric acid, 23 for sulfate).
 - *icomp_tr_all* has the size *ncomp* (number of all *possible* compounds).
 - *icomp_tr* has the size *mcomp(jm)* (number of all *simulated* compounds (per mode)).

The corresponding character array is *ccomp_tb*.

- *icompsel*: is an array of size *ncomp*, but in which all non-simulated species have a zero value. In the non-zero values, the *simulated* compounds are numbered from 1 to the number of simulated species. The command *icompsel(icompsel)* is used frequently throughout the code when the code is looping over e.g. *ncomp* (the total possible number of species) as this command will give a zero value if the species is not simulated (and thus can be easily cycled). It is thus an efficient way of selecting only the simulated species.

2) Species and mode dependent:

- *icompsel*: is a cumulative index which starts at 1 and counts over all *simulated* species per mode. A particular species e.g. SO₄mm will have a different *icompsel* value depending on the mode that it is in (e.g. *icompsel* SO₄mm mode NS may be 9 and mode KS it may be 15). *icompsel* values in each successive mode add to the values of the previous. *icompsel(jm)* has the size *mcomp(jm)*.
- The corresponding character array is *ccompsel_tr*, which tells you not only the species but also which mode it is in e.g. SO₄mm_ks or SO₄mm_as.
- *icompsel_all*: counts over all the possible compounds from 0 to the total number of compounds, but it counts cumulatively over the modes, thus the value for mode AS = value for mode KS + the number of species.

The actual values of the indices depends on the species simulated (i.e. on the setup of the *gmXe_parameter_script.inc* file), an example setup is given in Appendix 2.

6 Model Output

The model produces output in the form of netCDF files, which are written to the model working directory (the *WORKDIR*, set in the *xmessy* file). During a simulation, GMXe produces netCDF files with the general name *RESOLUTION_DATE_gmXe.nc*. These files contain the main aerosol parameters including; the aerosol dry radius, wet radius and number concentration.

The concentrations of the different species within the aerosol (and gas) phase are output in a netCDF file called *RESOLUTION_DATE_tracer_gp.nc*. The naming convention for the output arrays follows that used throughout the model; the modes are identified as NS, KS, AS etc and the cation / anion name is simply the chemical formula followed by the charge (e.g. SO₄MM for SO₄²⁻ and NH₄P for NH₄⁺).

7 References

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Appendix 1 – Example namelist setup

```
LGMXe = .T.
LOUTPUT = .T.
LMASS_DIAG = .F.
LSTRAT = .F.
LPSC = .F.
LNUCL = .T.
LCOND = .T.
LCOAG = .T.
LSIZE = .F.
LCOAT = .T.
LAH2O = .T.
LGH2O = .F.
LSHUM = .F.
LRAD = .T.
LACC = .F.
LCLC = .F.
LADYN = .F.
LCLWC = .F.
LCIWC = .F.
LCDNC = .F.
LICNC = .F.
LGAS = .T.
LAEROSOL = .T.
LNUMBER = .F.
LWETRAD = .T.
LDRYRAD = .T.
LDRYDENS = .T.
NLOWERMODE = 1
NUPPERMODE = 7
NEQM = 2
NNUCL = 1
LSKIP = .T.
LDRY = .F.
LSOLIDS = .T.
LRHDMIX = .F.
LHYSTER = .T.

l_calc_emis = T
l_tendency = F
l_seasalt = T
SSemis_stream = 'offlem'
SS_mass_as = 'emis_ss_m_as'
SS_num_as = 'emis_ss_n_as'
SS_mass_cs = 'emis_ss_m_cs'
SS_num_cs = 'emis_ss_n_cs'
l_direct_sulf = T
SO2emis_stream = 'offlem'
anth_emis_SO2 = 'anth_emis_SO2'
SO4_frac = 2.45
l_carbon = T
Cemis_stream = 'onlem'
emis_OC_insol = 'OC_sum_insol'
emis_OC_sol = 'OC_sum_sol'
emis_BC_insol = 'BC_sum_insol'
emis_N_insol = 'Num_insol'
emis_N_sol = 'Num_sol'
emis_N_insol_oc = 'Num_insol_oc'
emis_N_insol_bc = 'Num_insol_bc'
l_dust = T
Duemis_stream = 'offlem'
emis_dust = 'emis_dust'
TropopStream = 'tropop'
TropopIndex = 'tp_i'
PscStream = 'psc'
Pscreg = 'PSC_region'
driver_call = 'physc'
rad_diag_wavelen = 0.55,1.0
```

Appendix 2 – Summary of index naming

Example setup of the indices, calculated by the model. The actual numbers depend on the choice of species simulated. This information is also written to the log file during each run.

Mode	ccomp_tb	icomp_tr	ccomp_tr	icomp	icomp	ccomp
0	H2SO4	2	H2SO4	1	2	awhsa
0	HNO3	4	HNO3	2	4	awhna
0	HCl	5	HCl	3	5	awhca
0	H2O	10	H2O	4	10	awh2o
0	NH3	43	NH3	5	43	awxam
1	H2O	10	H2O_ns	6	66	awh2o
1	Hp	15	Hp_ns	7	71	ncihy
1	NH4p	16	NH4p_ns	8	72	nciam
1	SO4mm	23	SO4mm_ns	9	79	naisu
1	HSO4m	24	HSO4m_ns	10	80	naihs
1	NO3m	25	NO3m_ns	11	81	naino
1	OHm	31	OHm_ns	12	87	naioh
2	H2O	10	H2O_ks	13	122	awh2o
2	Hp	15	Hp_ks	14	127	ncihy
2	NH4p	16	NH4p_ks	15	128	nciam
2	SO4mm	23	SO4mm_ks	16	135	naisu
2	HSO4m	24	HSO4m_ks	17	136	naihs
2	NO3m	25	NO3m_ks	18	137	naino
2	OHm	31	OHm_ks	19	143	naioh
2	OC	38	OC_ks	20	150	awxfa
2	BC	39	BC_ks	21	151	awxlg
3	H2O	10	H2O_as	22	178	awh2o
3	Hp	15	Hp_as	23	183	ncihy
3	NH4p	16	NH4p_as	24	184	nciam
3	SO4mm	23	SO4mm_as	25	191	naisu
3	HSO4m	24	HSO4m_as	26	192	naihs
3	NO3m	25	NO3m_as	27	193	naino
3	OHm	31	OHm_as	28	199	naioh
3	SS	36	SS_as	29	204	awscl
3	DU	37	DU_as	30	205	awcsu
3	OC	38	OC_as	31	206	awxfa
3	BC	39	BC_as	32	207	awxlg
4	H2O	10	H2O_cs	33	234	awh2o
4	Hp	15	Hp_cs	34	239	ncihy
4	NH4p	16	NH4p_cs	35	240	nciam
4	SO4mm	23	SO4mm_cs	36	247	naisu
4	HSO4m	24	HSO4m_cs	37	248	naihs

4	25	naino	NO3m	25	1	38
4	OHm	31	OHm_cs	39	255	naioh
4	SS	36	SS_cs	40	260	awscl
4	DU	37	DU_cs	41	261	awcsu
4	OC	38	OC_cs	42	262	awxfa
4	BC	39	BC_cs	43	263	awxlg
5	H2O	10	H2O_ki	44	290	awh2o
5	Hp	15	Hp_ki	45	295	ncihy
5	NH4p	16	NH4p_ki	46	296	nciam
5	SO4mm	23	SO4mm_ki	47	303	naisu
5	HSO4m	24	HSO4m_ki	48	304	naihs
5	NO3m	25	NO3m_ki	49	305	naino
5	OHm	31	OHm_ki	50	311	naioh
5	OC	38	OC_ki	51	318	awxfa
5	BC	39	BC_ki	52	319	awxlg
6	H2O	10	H2O_ai	53	346	awh2o
6	Hp	15	Hp_ai	54	351	ncihy
6	NH4p	16	NH4p_ai	55	352	nciam
6	SO4mm	23	SO4mm_ai	56	359	naisu
6	HSO4m	24	HSO4m_ai	57	360	naihs
6	NO3m	25	NO3m_ai	58	361	naino
6	OHm	31	OHm_ai	59	367	naioh
6	DU	37	DU_ai	60	373	awcsu
7	H2O	10	H2O_ci	61	402	awh2o
7	Hp	15	Hp_ci	62	407	ncihy
7	NH4p	16	NH4p_ci	63	408	nciam
7	SO4mm	23	SO4mm_ci	64	415	naisu
7	HSO4m	24	HSO4m_ci	65	416	naihs
7	NO3	25	NO3m_ci	66	417	naino
7	OHm	31	OHm_ci	67	423	naioh
7	DU	37	DU_ci	68	429	awcsu