AeroTab6 User's Guide

Alf Kirkevåg

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1 Introduction

We refer to the online aerosol module in NorESM as OsloAero, and to the offline size-resolving aerosol microphysics model that produces look-up tables (LUT) for use in NorESM as AeroTab. AeroTab, including table look-ups and interpolations with respect to aerosol–radiation (optical properties) and aerosol–cloud interaction calculations (aerosol size parameters) in OsloAero, was first developed and described by Kirkevåg, Iversen, and Dahlback (1999) and Kirkevåg and Iversen (2002), with some updates by Kirkevåg et al. (2005). Later versions of both components of the production-tagged aerosol module as a whole are described by Seland et al. (2008) and Kirkevåg et al. (2008), Kirkevåg et al. (2013) and (Kirkevåg et al., 2018). Additional updates specifically for NorESM2 are described by Seland et al. (2020) and Olivié et al. (in prep.). A new AeroTab feature as of February 2020 is the optional simplified treatment of how size distributions change as they age and grow by hygroscopic swelling. Since this is not previously published, it will be described in some detail in section 3.3.

Note that while aerosol hygroscopicity with respect to sub-saturated conditions for use in the optics calculations is calculated within AeroTab, hygroscopicity for supersaturated conditions is not. This is because the aerosol activation code in NorESM (Abdul-Razzak and Ghan, 2000) does not require size-resolved hygroscopicity information, only the mean hygroscopicity for each mode/mixture as a whole. AeroTab instead provides look-up tables of aerosol dry size parameters (modal median radius and standard deviation when fitted to a lognormal distribution) for each of the modes, which together with the hygroscopicities calculated online in OsloAero are used to determine what number fraction (for each of the modes) is activated as CCN in NorESM.

AeroTab is not only a tool for producing LUT for NorESM. It is also used in case studies of aerosol growth by different microphysical processes (which are already treated in OsloAero, or under consideration to include) and subsequent impacts on aerosol size distributions and size-integrated optical parameters such as extinction and absorption, or mass specific extinction (MEC) and absorption, asymmetry factor, single scattering albedo and back-scattering. There are strong links to NorESM through the common assumption that the aerosol module is of the "production-tagged" type (Kirkevåg et al., 2018), and the fact

that the wavelengths for which the optics calculations are made, are tailored to the wavelength bands used in various versions of NorESM, i.e. as in CAM4 (CAMRT) or in CAM5 and later versions (RRTMG). However, AeroTab may be modified to produce LUT for other models as well. E.g., an AeroTab version for the EMEP model exists and LUT for optical properties have been produced, but not yet tested in model runs.

The version of AeroTab and NorESM used as basis for this document is a post-CMIP6 version AeroTab6 (identical to the CMIP6 version except for some additional functionality described in section 3.3) and the CMIP6 version of the Norwegian Earth System Model, NorESM2 (Seland et al., 2020; Olivié et al., in prep.). The version number 6 is used to indicate that this version of AeroTab is tailored for use with CAM6-Nor, the atmospheric model in NorESM2. For simplicity and brevity, the names AeroTab and NorESM are hereafter used throughout the text, and similar for OsloAero. Older versions share many of the same features, but differ in others.

2 How to obtain, build and run the model

AeroTab is a part of the NorESM repository on github, located in the folder

components/cam/tools/AeroTab

In its present form the model does not depend on any other parts of NorESM, and is run separately (offline). You may want to move the code to a different location or platform. Copy (e.g., scp -r) the entire AeroTab directory, for instance to your local PC. To build the model, which is written in fortran, run

make

The Makefile then creates the executable "AeroTab", which on a Linux platform is run interactively by

./AeroTab

In the first tests you will probably prefer to configure AeroTab so that it does not produce a whole set of look-up tables (LUT), which may take many hours. How to edit the code for this purpose will be described in section 4.

3 AeroTab code and required input data

The AeroTab code consist of 26 fortran files, of which 24 has the ".f" extension and the remaining 2 (which are modules) use the extension ".F90", as listed in the Makefile. The input files to the code are all found under the AeroTab/input folder.

3.1 Input data

There are two types of input to the AeroTab code. The first type (the .inp files) consists of spectrally resolved complex refractive indices for each aerosol component treated in NorESM, including water vapour. Not all the files are used. Which ones that are presently (or for whatever version of the code you have) in use can be seen from the hard coded file-names in tabrefind.f. The other .inp files are either from older AeroTab versions or for testing purposes. These input files have headers explaining their content, including references.

One additional file (xtspec.dat) contains spectrally resolved solar irradiances at top of the atmosphere (TOA), for use in the code for Chandrasekhar averaging over spectral bands.

The many .txt files are not used as input directly, but give refractive index values for mineral dust from diferent stations as reported by Di Biagio et al. (2017), see also Olivié et al. (in prep.). A multi-site average has been calculated from these and stored in mineral_nymix.inp.

3.2 The standard AeroTab version

The standard code version, used in CMIP6, is an AeroTab version with full complexity with respect to size resolved number and mass concentration distribution within each mixture (often referred to as mode) of the multi-modal aerosol distribution treated in NorESM2. The code for this version is as defined by the following list of fortran code files. The tab indents indicate how far down the respective subroutines (or modules used) are on the call tree, and the order reflects how early they are called (or use'ed for modules) the first time. One additional subroutine is found in the chandrav.f file itself, as indicated in blue below.

AeroTab.f
  commondefinitions.F90 (module)
    shr_kind_mod.F90 (module)
  specbands.f
  constsize.f
  modepar.f
  drydist.f
  condsub.f
  coagsub.f
  tabrefind.f
  hygro.f
  openfiles.f
  tableinfo.f
  conteq.f
    smolar.f
  rhsub.f
    koehler.f

mixsub.f
modetilp.f
sizemie.f
refind.f
miev0.f
chandrav.f → chsub

AeroTab.f contains the main program **AeroTab** which loops over a predefined (multidimensional) discrete input parameter space to produce look-up tables (LUT). The module **shr_kind_mod** defines various precision/kind constants and makes them public within AeroTab.

The module **commondefinitions** defines the aerosol types and some of their physical properties, such as mass densities and other parameters needed for calculation of hygroscopicities. It also presets the assumed modal mean radius and standard deviation for a log-normal size distribution for each of the mixtures (or modes, as treated in OsloAero) at the point of emission/production, i.e. prior to any growth. This module is found in the OsloAero code as well, and should be identical to that. AeroTab and OsloAero are not (yet) coupled so that the same file is automatically used, but the OsloAero code (see comments on this in opttab.F90) which reads the LUT can easily be modified to produce an error message if it finds contradictive information based on its own **commondefinitions** and the corresponding information found in the header of each LUT (already implemented in AeroTab).

specbands defines the spectral bands, corresponding to spectral bands in the radiative transfer code in NorESM, and sub-bands used for Chandrasekhar averaging (a weighting with the solar spectral flux at TOA) over bands that are so wide that the mid-band wavelength is thought not to be representative for the band as a whole, with respect to gross aerosol optical properties.

constsize defines or determines mathematical and physical constants needed in AeroTab, such as diffusion coefficients and thermal velocities of the condensable gases. It furthermore calculates the mid and end radii of each size bin used in AeroTab, and the size dependent mass density of the agglomarate (fractal) BC mode from fossil fuel combustion (the OsloAero tracer BC_AX), which is a special case in this respect.

modepar defines parameters and arrays for the various mixtures which in AeroTab are numbered kcomp = 0, 1, 2,... , 10. Assumed values for mixture specific parameters such as the accomodation coefficients (alpha) are given here, as well as arrays for how much total mass from condensation, coagulation and cloud processing that is allowed to become internally mixed with the background particles (assuming normalized size modes of 1 particle per cm^3). These arrays are named catote (size = 16) for kcomp = 1 - 4 and catot (size = 6) for kcomp = 5 - 10. Here is also defined a set of common (for all kcomp values) arrays of input values concerning the composition and production origin of added mass; namely the mass fraction of internally mixed mass which is carbonaceous (BC and/or OM), fac (size = 6); how much of the added carbonaceous mass comes as BC, fbc (size = 6); and how much of the added sulfate (the mass fraction

1-fac) which comes from wet phase chemistry (cloud processing), faq (size = 6). Additionally, frombg (size = 6) denotes the OM fraction in the background mode for kcomp = 1 (consisting of sulfate and/or SOA), and frbcbg (size = 6) is the BC fraction in the background mode for kcomp = 4 (consisting of OM and BC). Finally there is an array for the ambient relative humidity, relh (size = 10). The corresponding arrays in OlsoAero (in opttab.F90) are named cate, cat, fac, faq, fbc, fombg, fbcbg, and rh, respectively.

drydist calculates the dry background number size distribution for the mixture (kcomp) and its size integrated mass concentration (for a normalized size mode of 1 particle per cm^3).

condsub calculates the radius dependent diffusion coefficients for sulfate or SOA.

coagsub calculates the radius dependent Brownian coagulation coefficient for mono-disperse fine mode particles. Here the size dependency refers to the radii of the particles onto which these smaller particles are assumed to coagulate.

tabrefind calculates (by interpolation in the input files) wavelength dependent complex rafractive indices for each of the aerosol components.

hygro calculates hygroscopic properties for each of the pure aerosol components (externally mixed).

openfiles opens the (empty) LUT files and makes them writable.

tableinfo adds header information for the LUT files. This includes an explanation of what the files contain, and information which facilitates checking of important input-info assumed in AeroTab against OsloAero (to make sure that this particular LUT is compatible with the OsloAero version which is being used).

conteq calculates the modified dry size dependent number and mass distributions, taking into account how sulfate, OM and BC are internally mixed with the background aerosol, based on the production mechanisms involved. The numerical method used is based on Smolarkiewicz (1983).

smolar is the the anti-diffusive part of the Smolarkiewicz scheme which is used to solve the continuity equations for aerosol number and component specific mass concentration as function of size.

rhsub calculates the modified wet size dependent number and mass distributions, taking into account how the hygroscopicity for internally and externally mixed aerosol varies with size based on the production mechanisms involved. The Smolarkiewicz upwind scheme is applied also here.

koehler solves the Köhler equation and finds the radius dependent hygroscopic growth factor at a given ambient relative humidity RH.

mixsub calculates (by use of volume mixing) hygroscopic properties for an internal mixture of aerosol components, using the component specific hygroscopicites found in hygro.

modetilp calculates (by use of a least squares fitting method) modal parameters for a log-normal size distribution with best fit to the non-lognormally distributed modified dry size distribution.

sizemie calculates the spectral aerosol optical parameters by calling the Mie code for each size bin, and then integrating over all sizes. If AeroTab is

configured to take out AeroCom diagnostics, aerosol extinction and absorption is also calculated (and tabulated in the AeroCom LUT) for particle radii $< 1\mu$m, see section 5.2).

refind calculates complex refractiv indices for an internal mixture of aerosol components, based on the component specific refractive indices found in tabrefind. The method used is simple volume mixing for all components (including water) except BC. For mixing of BC with the rest, the Maxwell Garnett mixing rule is applied (see Kirkevåg et al., 2005).

miev0 is the Mie code, originally made by Warren J. Wiscombe (wiscombe@climate.gsfc.nasa.gov, see references in the code file).

chandrav calculates the Chandrasekhar averaged optical parameters for the widest wavelength bands.

chsub carries out the Chandrasekhar weighting of optical parameters with the read in spectrally resolved TOA irradiance.

3.3 The AeroTab light version

The light version of AeroTab is the same as the standard version except for the 3 subroutines marked in red below, conteqlight.f, rhsublight.f and modetilplight.f, which replace the standard code files conteq.f, rhsub.f and modetilp.f. The simplifying assumptions are that all internal mixing is homogeneous with respect to size (within a mixture/mode, kcomp), regardless of production mechanism, and that the modified number size distributions including growth remain log-normal. As in the aerosol microphysics schemes in CESM2 (e.g. MAM3), we let the median modal radius change while keeping the standard deviation constant.

AeroTab.f
- commondefinitions.F90 (module)
  - shr_kind_mod.F90 (module)
- specbands.f
- constsize.f
- modepar.f
- drydist.f
- condsub.f
- coagsub.f
- tabrefind.f
- hygro.f
- openfiles.f
- tableinfo.f
- conteqlight.f
  - smolar.f
- rhsublight.f
  - koehler.f
    - mixsub.f
- modetilplight.f
- sizemie.f

refind.f
miev0.f
chandrav.f → chsub

conteqlight calculates the modified dry size dependent number and mass distributions by use of simple, analytical formulas based on conservation of mass and number.

rhsublight calculates the modified wet size dependent number and mass distributions, assuming that the hygroscopicity of an externally or internally mixed aerosol does not vary with size.

modetilplight tabulates the modal standard deviation and the median radius for the modified log-normal size distribution (calculated in conteqlight).

Since the AeroTab light version is not previously published, a more detailed description of what is new (simplified) compared to the standard (more complex) AeroTab version is presented here.

The number size distribution (normalized to 1 particle per cm^3) for aerosols in mixture k (called *kcomp* in the code) at the point of emission or production is lognormal in both AeroTab versions:

$$\frac{dN_k}{d\log r} = \frac{1}{\sqrt{2\pi}\log\sigma_k}\cdot\exp[-\frac{1}{2}\left(\frac{\log(r/R_k)}{\log\sigma_k}\right)^2], \tag{1}$$

where R_k and σ_k are the number median modal radius and standard deviation of mixture/mode k, respectively. Here log means $\log_{10}$, but since $\ln x = \ln 10 \cdot \log x$, Eq. 1 is equivalent to that obtained by replacing "log" by "ln" everywhere in the equation. Integration of particle volume over all radii r yields total volume

$$V_k = \frac{4}{3}\pi R_k^3 \cdot \exp\left[\frac{9}{2}\left(\ln\sigma_k\right)^2\right]. \tag{2}$$

Now, let the original particle distribution with total volume $V_{k,0}$ (from Eq. 2) become homogeneously internally mixed with condensate, coagulate and cloud processed aerosol with volume $V_{k,add}$. Since σ_k is assumed to remain unchanged, the modified number size distribution in AeroTab light (**conteqlight**) is simply given by Eq. 1, but with a modified modal mean radius

$$R_k^{mod} = R_k \cdot \sqrt[3]{(V_{k,0} + V_{k,add})/V_{k,0}}. \tag{3}$$

For hygroscopic growth, added condensate in the form of water yields a increase in all particle radii of $f_g = r_{wet}/r_{dry}$. Since the growth factor f_g varies with size even for homogeneously mixed particles, we here (in **rhsublight**) chose to use the f_g value calculated at the modal median radius (R_k^V) of the corresponding *volume* size distribution, which is given by (see e.g. Eq. 7.52 in Seinfeld and Pandis, 1998)

$$R_k^{V,mod} = 0.5 \cdot \exp[(\ln(2R_k^{mod}) + 3(\ln\sigma_k)^2]. \tag{4}$$

Just like in the standard AeroTab code (in **rhsub**), f_g (at $r = R_k^{V,mod}$) is calculated by solving the Köhler equation for a given ambient relative humidity.

Unlike the standard AeroTab treatment (in **modetilp**), the modified dry number size distributions are here already lognormal. Hence no lognormal fitting is needed, and the modal median standard deviation σ_k and modified median radius R_k^{mod} (from **conteqlight**) can be tabulated directly (in **modetilplight**).

Figure 1 shows an example of how size distributions and component volume fractions as function of size may look like with the two different AeroTab versions. In Figure 2 we see the resulting wavelength dependent optical parameters (for use in NorESM) from the different AeroTab versions, calculated for modified mixtures (aged aerosols) from the same example as in Figure 1.

4 AeroTab configuration/setup

Before the main code with multiple do loops (over $kcomp$, $irelh$, $ictote$, $ifbcbg$, $ifac$, $ifbc$, and $ifaq$), AeroTab.f has a configuration section following the comment "Modify the following input to create different sets of look-up tables".

First of all, here you can choose

$iopt = 0$ or $iopt = 1$,

Setting the value to 1 configures the code to create optics look-up tables (LUT) by calling **sizemie**, while $iopt = 0$ instead tells it to calculate lognormnal fits of the (generally non-lognormal) modified size distributions by calling **modetilp** or **modetilplight**. Regardless of the choice of $iopt$, the calculation of size distributions of particle number and mass concentrations for the modified aerosol are needed (from **conteq** or **conteqlight**). If $iopt = 0$, however, only the dry cases ($RH = 0\%$) are needed, i.e. $irelh = 1$.

The next configuration parameter is the number of wavelength bands (ib) which we want the optical parameters to be calculated for. Here the following options are available:

$ib = 31$ (or $ib = 29$) or $ib = 19$,

where $ib = 31$ and $ib = 19$ yield optics look-up tables (LUT) which are adapted to the short-wave (SW) and long-wave (LW) parts of RRTMG (used in NorESM1.2 and NorESM2), respectively, while $ib = 29$ instead yields optics LUT adapted to the SW part of CAMRT (used in NorESM1). The NorESM1 option $ib = 29$ has not been tested for the present AeroTab version, and should not be used without great caution. Since the spectral bands and corresponding radiation code is only one of many changes since NorESM1, please check out and use the AeroTab version that came with that specific model version if you need to produce new LUT for use in NorESM1.

The final configuration option for standard use of AeroTab (to produce LUT for NorESM) is the choice between a version with full complexity (used in CMIP6) and a simplified version, already described in Sect. 3.3:

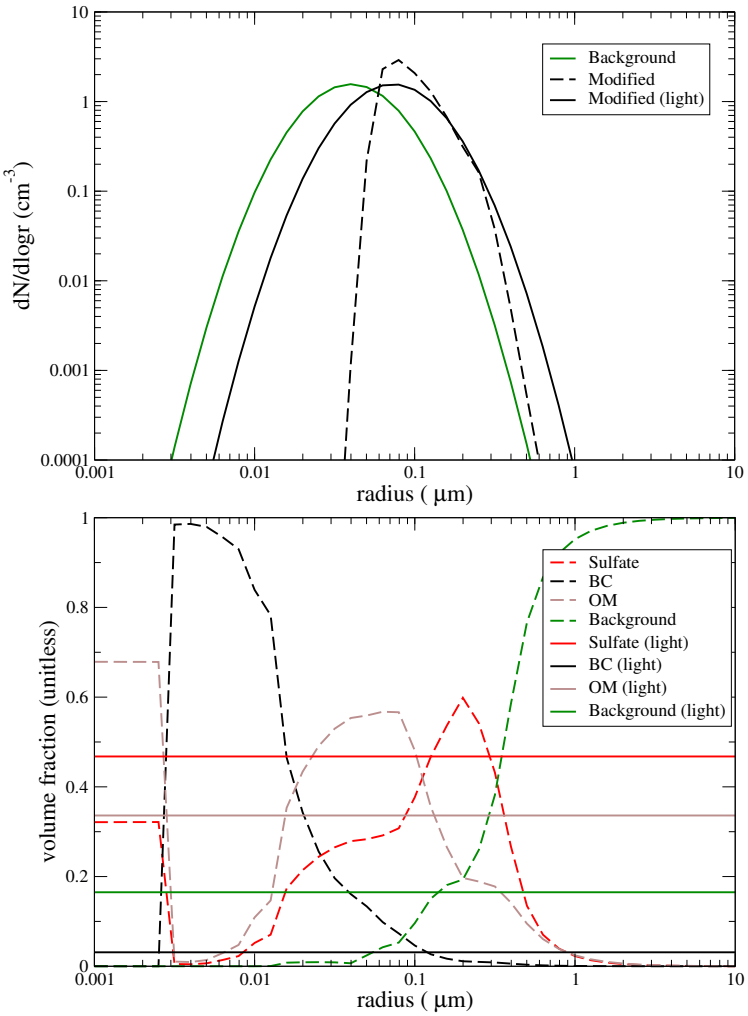

Figure 1: Aerosol number distributions and component volume fractions as functions of size with two different AeroTab versions, for an example where the Aitken mode OM&BC has been modified by condensation, coagulation and cloud processing. For comparison, also the original background size distribution is shown in the upper panel. The figures are made with the following combination of input indices in AeroTab.f: $kcomp = 4$, $irelh = 1$, $ictote = 8$, $ifbcbg = 3$, $ifac = 3$, $ifbc = 2$, and $ifaq = 4$. In this case the background mode consists of a homogeneous mixture of OM and BC, and the relative humidity is zero, so that there is no hygroscopic growth. The discontinuous behaviour of the volume fractions at very small radii are due to numerical errors (a more exact solution would require too many iterations and too much CPU time), but only occur for sizes where the number and mass of particles is so small that any impacts on CCN and opical properties are insignificant. Curves labeled "(light)" are from the light version of AeroTab.

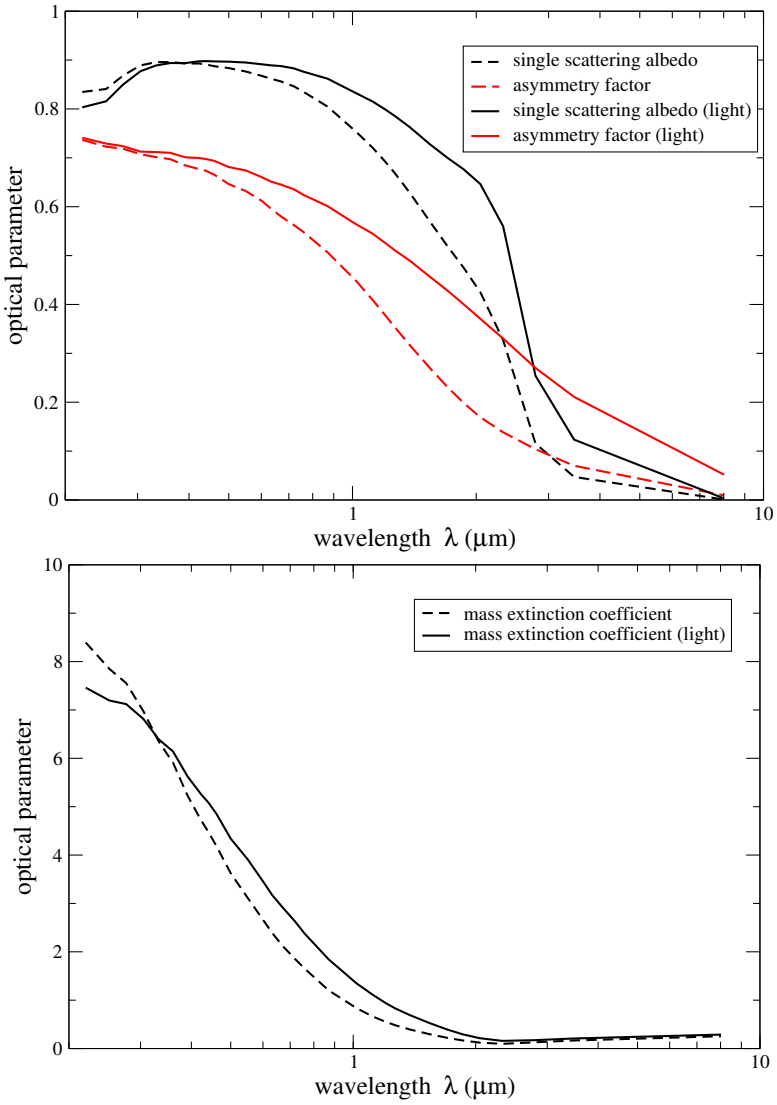

Figure 2: Size-integrated (gross) dry aerosol optical parameters as functions of wavelength for the two different AeroTab versions (or to be more precise, configurations), for the same example as in Fig 1. Only results for the aged aerosol are shown. Curves labeled "(light)" are from calculations with the light version of AeroTab.

$light = .true.$ or $light = .false.$

The AeroTab light version is much faster to run. On my (old) PC it takes approximately 10 minutes to produce all the required LUT for NorESM, compared to more than a day with the standard version. This does not make NorESM faster, however, since the complexity with respect to the "production tagged" input to the LUT (the number of dimensions) is the same as in the standard version. For any extensive use of AeroTab light in the future, it is recommended to simplify both the structure of the LUT and the corresponding NorESM code, i.e. the table look-ups and interpolations. As a start, this can be done by removing redundant information in the input to the LUT. E.g., in AeroTab light there is no need to distinguish between BC from coagulation and BC in the background mode, since BC is distributed homogeneously (no radius independence). The same must then be done in the OsloAero code of NorESM. This involves changes to a number of subroutines and modules (see Sect. 7.2).

Further configuration settings are not necessary for the LUT calculations, but may be practical for testing and plotting of output for special cases, or if you only need to produce LUT for one or a few mixtures ($kcomp$). The choice of taking out, or not, extra diagnostics from intermediate calculations of size-dependent distributions of particle number and component volume fractions, as well as wavelength dependent optical parameters, is made by setting

$extradiag = .true.$ or $extradiag = .false.$

This is described in more detail in Sect. 6.

Furthermore, in order to run the code for only mixture k, for example, just change the outer do loop in AeroTab.f from

do $kcomp = 0, 10$ to do $kcomp = k, k$

Similarly, if you only want to run calculations for dry aerosols (no hygroscopic growth), you may change the next do loop from

do $irelh = irelh1, irelh2$ to do $irelh = 1, 1$

More generally, if we are interested in specific combinations of input variables for a given mixture, e.g. in order to make a figure like Fig. 1, we may edit all the upper and lower bounds of the input variable indices in the inner "do loops", namely $irelh$, $ictote$, $ictot$, $ifbcbg$, $ifac$, $ifbc$, and $ifaq$. The corresponding arrays (and array sizes) for input to each of the LUT, as defined in **modepar**, are $relh(10)$, $ctote(16)$, $ctot(6)$, $frbcbg(6)$, $frac(6)$, $frabc(6)$, and $fraq(6)$, see Sect. 3.2. Any changes to the preset values of these arrays can be done in modepar.f. Note that if such changes are done for a new set of LUT to be used in NorESM, the respective arrays in OsloAero must be edited accordingly, see Sect. 7.2.

5 Look-up tables (LUT) and their structure

All look-up tables (LUT) produced with AeroTab are ASCII files with headers which explain their content. Details about their content and structure follows below. Note that there are purely extarnal mixtures in NorESM which *apparently* do not correspond directly to the look-up tables listed below, namely those numbered 12 and 14 (11 and 13 are no longer used). The physical properties of these mixtures are however found from the corresponding internal mixtures numbered 2 and 4, for the special case where no (or insignificant amounts) of added mass from condensation, coagulation or cloud processing is present, i.e. with zero added aerosol mass onto the background mode/mixture.

Configured with $iopt = 0$ and otherwise no code changes, AeroTab produces the following output files which can be used as LUT in NorESM:

logntilp1.out
logntilp2.out
logntilp3.out
logntilp4.out
logntilp5.out
logntilp6.out
logntilp7.out
logntilp8.out
logntilp9.out
logntilp10.out

Henceforth we will use the short form logntilp$k$.out, where $k = 1 - 10$, k being the mixture identifying number (called *kcomp* in the code). This set of LUT contains the size parameters modified median radius R_k^{mod} and standard deviation σ_k^{mod} for the lognormal fits to the generally non-lognormal size distributions (from **modetilp**), or R_k^{mod} and σ_k (directly from **conteqlight**) when the AeroTab light version is used. No logntilp0.out file is produced, since this mixture ($kcomp = 0$) has a prescribed lognormal size distribution, so that no look-ups and interpolations in OsloAero are needed.

The strucure of the LUT varies depending on the complexity of the internal mixture. In logntilp$k$.out for $k = 1 - 3$ (where $k = 3$ is not used in NorESM2), the stored information below the header is on the form

$kcomp$, $catot$, fac, R^{mod}, $log_{10}\sigma^{mod}$

where the output variables are written in purple for clarity. As explained in the header, $kcomp$ is the aerosol mixture number, $catot$ (which for $k = 1 - 4$ is named $catote$ in AeroTab.f) is total added internally mixed mass ($\mu g/m^3$) to the normalized background mode, and fac is the OM mass fraction of $catot$ (consisting of OM and sulfuric acid, H_2SO_4). Note that the fitted modal median radius R^{mod} and standard deviation σ^{mod} do not depend on $fombg$ (the OM fraction in the background OM and BC mass for $kcomp = 1$), since it does not change the number size distribution. The optical properties do depend on

$fombg$, however, see below.

In logntilp4.out the stored information below the header is on the form

$kcomp$, $catot$, fac, faq, R^{mod}, $log_{10}\sigma^{mod}$

where the additional input variable faq is the mass fraction of wet phase produced sulfate, present as ammonium sulfate, $(NH_4)_2SO_4$, of the total added sulfate (with concentration $catot * (1 - fac)$).

In logntilp$k$.out for $k = 5 - 10$ the stored information below the header is on the form

$kcomp$, $catot$, fac, fbc, faq, R^{mod}, $log_{10}\sigma^{mod}$

where the additional input variable fbc is the mass fraction of BC to total added OM and BC (with concentration $catot * fac$).

Configured with $iopt = 1$ and $ib = 31$ and otherwise no code changes, AeroTab produces the following LUT files for SW aerosol optical parameters (the first two rows) and other size range specific parameters for dry aerosols (the third row):

kcomp0.out	aerocomk0.out	aerodryk0.out
kcomp1.out	aerocomk1.out	aerodryk1.out
kcomp2.out	aerocomk2.out	aerodryk2.out
kcomp3.out	aerocomk3.out	aerodryk3.out
kcomp4.out	aerocomk4.out	aerodryk4.out
kcomp5.out	aerocomk5.out	aerodryk5.out
kcomp6.out	aerocomk6.out	aerodryk6.out
kcomp7.out	aerocomk7.out	aerodryk7.out
kcomp8.out	aerocomk8.out	aerodryk8.out
kcomp9.out	aerocomk9.out	aerodryk9.out
kcomp10.out	aerocomk10.out	aerodryk10.out

The content and structure of the aerocom$k$.out and aerodry$k$.out files, which are only utilized by NorESM when configured to do so, will be described in more detail in Sect. 5.2.

In kcomp0.out the stored information below the header is on the form

$kcomp$, $iband$, rh, SSA, g, β_{ext}, k_{ext}

where $iband$ is the wavelength band number (1-14), rh is the ambient relative humidity (unitless), SSA is the single scattering albedo (unitless), g is the asymmetry factor (unitless), β_{ext} is the extinction coefficient (km^{-1}), and k_{ext} is the mass specific extinction coefficient (m^2g^{-1}). Note that while the more often used MEC (mass extinction coefficient) is defined as the extinction per unit dry aerosol mass, k_{ext} is the extinction per unit humidified aerosol aerosol mass, i.e. including the internally mixed water from hygroscopic growth. Note also that the number of bands here (14), which corresponds directly to the SW spectral bands in RRTMG (in NorESM2) is different from ib, which is the total

number of original spectral bands before the Chandrasekhar averaging.

In kcomp1.out the stored information below the header is on the form

$kcomp$, $iband$, rh, $fombg$, $catot$, fac, SSA, g, β_{ext}, k_{ext}

where the additional input variables $fombg$, $catot$ and fac are as explained above for logntilp1.out.

In kcomp2.out (and kcomp3.out, not used in NorESM2) the stored information below the header is on the form

$kcomp$, $iband$, rh, $catot$, fac, SSA, g, β_{ext}, k_{ext}

In kcomp4.out it is on the form

$kcomp$, $iband$, rh, $fbcbg$, $catot$, fac, faq, SSA, g, β_{ext}, k_{ext}

and finally in kcomp$k$.out (for $k = 5 - 10$) it is on the form

$kcomp$, $iband$, rh, $catot$, fac, fbc, faq, SSA, g, β_{ext}, k_{ext}

where all input variables are defined as explained above for logntilp$k$.out.

Configured with $iopt = 1$ and $ib = 19$ and otherwise no code changes, AeroTab instead produces the following LUT files for LW aerosol optical parameters:

lwkcomp0.out
lwkcomp1.out
lwkcomp2.out
lwkcomp3.out
lwkcomp4.out
lwkcomp5.out
lwkcomp6.out
lwkcomp7.out
lwkcomp8.out
lwkcomp9.out
lwkcomp10.out

These LUT files have the exact same input parameters as do kcomp$k$.out, but only one output variable, the wavelength dependent mass specific absorption coefficient ($m^2 g^{-1}$) for the LW radiation code, k_{abs}. This is the only LW optical parameter required as input to RRTMG in NorESM2. The structure of these LUT files is therefore much the same as for kcomp$k$.out, apart from the smaller number of output variables. E.g., in lwkcomp5.out the stored information below the header is on the form

$kcomp$, $iband$, rh, $catot$, fac, fbc, faq, k_{abs}

and similar for the LW optics LUT for the other mixtures.

5.1 LUT for the standard NorESM2 configuration

Look-up tables which are used in NorESM2 whenever it is configured with the default OsloAero module (the alternative being either of the modal schemes of CESM, such as MAM3), are the following:

logntilp$k$.out, where $k = 1 - 10$
kcomp$k$.out, where $k = 0 - 10$
lwkcomp$k$.out, where $k = 0 - 10$

The content and structure of these LUT files are as described above. As also described, these LUT files contains essential information connecting the aerosol microphysics to CCN activation and optical properties, both of which have impacts on radiative transfer in NorESM2.

5.2 LUT for the AeroCom configuration of NorESM2

If NorESM2 is configured with "#define AEROCOM" (e.g., in preprocessorDefinitions.h), the following LUT are also utilized:

aerocomk$k$.out, where $k = 0 - 10$
aerodryk$k$.out, where $k = 0 - 10$

These files contain a larger number of output parameters than the default LUT described above. This particular set of diagnostics is originally based on requirements for model output data for submision to the AeroCom database for use in AeroCom studies (see e.g, https://aerocom.met.no/protocol.html), but are useful for aerosol specific diagnostics in general, and for use with the ModIvsModII scripts in particular. The ModIvsModII scripts, which compare two different sets of NorESM simulations side by side in figures, are found under /components/cam/tools/diagnostics/ncl/ ModIvsModII/ in the NorESM github repository. The aerocomk$k$.out files contain optical parameters for specific wavelengths and size ranges, while the aerodryk$k$.out files contain size-integrated information on the dry aerosol mass, volume and surface areas.

Just as for the default LUT files, the structure of these files varies depending on the complexity of the mixture. In aerocomk0.out, which applies for a purely external mixture, the stored information below the header (which as usual includes a description of the content) is on the form

$$kcomp,\ rh,\ \beta^{bg}_{ext,440},\ \beta^{bg}_{abs,440},\ \beta^{bg}_{ext,500},\ \beta^{bg}_{abs,500},\ \beta^{bg}_{abs,550},$$

$$\beta^{bg}_{ext,670},\ \beta^{bg}_{abs,670},\ \beta^{bg}_{ext,870},\ \beta^{bg}_{abs,870},\ \beta^{bg,d<1\mu m}_{ext,550},\ \beta^{bg,d>1\mu m}_{ext,550},\ \beta^{bg}_{back,550}$$

Here the 9 first output parameters are extinction (ext) and absorption (abs) coefficients for the background particles (bg), which in this case is the same as the mixture itself, at wavelengths 440, 500, 550, 670 and 870 nm. $\beta^{bg}_{ext,550nm}$ is omitted in the first line because it can be calculated as the sum of $\beta^{bg,d<1\mu m}_{ext,550nm}$

and $\beta_{ext,550nm}^{bg,d>1\mu m}$, the extinction coefficients (at 550 nm) for particle diameters below and above 1 μm, respectively. The last output parameter, $\beta_{back,550nm}^{bg}$, is the back-scattering (at 180°) coefficient at wavelength 550 nm, with unit $km^{-1}sr^{-1}$. All the other output parameters have unit km^{-1}.

In aerocomk1.out, which applies for an internal mixture, the stored information below the header is instead on the form

$kcomp$, rh, $fombg$, $catot$, fac, $\beta_{ext,440}$, $\beta_{ext,500}$, $\beta_{ext,670}$, $\beta_{ext,870}$,

$\beta_{ext,440}^{bg}$, $\beta_{ext,500}^{bg}$, $\beta_{ext,670}^{bg}$, $\beta_{ext,870}^{bg}$, $\beta_{ext,440}^{bc}$, $\beta_{ext,500}^{bc}$, $\beta_{ext,670}^{bc}$, $\beta_{ext,870}^{bc}$,

$\beta_{ext,440}^{om}$, $\beta_{ext,500}^{om}$, $\beta_{ext,670}^{om}$, $\beta_{ext,870}^{om}$, $\beta_{ext,440}^{su}$, $\beta_{ext,500}^{su}$, $\beta_{ext,670}^{su}$, $\beta_{ext,870}^{su}$,

$\beta_{abs,440}$, $\beta_{abs,500}$, $\beta_{abs,550}$, $\beta_{abs,670}$, $\beta_{abs,870}$, $\beta_{ext,550}^{bg,d<1\mu m}$, $\beta_{ext,550}^{bg,d>1\mu m}$,

$\beta_{ext,550}^{bc,d<1\mu m}$, $\beta_{ext,550}^{bc,d>1\mu m}$, $\beta_{ext,550}^{om,d<1\mu m}$, $\beta_{ext,550}^{om,d>1\mu m}$, $\beta_{ext,550}^{su,d<1\mu m}$, $\beta_{ext,550}^{su,d>1\mu m}$,

$\beta_{back,550nm}$, $\beta_{abs,550nm}^{bg}$, $\beta_{abs,670nm}^{bc}$, $\beta_{abs,550nm}^{om}$, $\beta_{abs,550nm}^{su}$

The new output parameters relative to those for aerocomk0.out above, $\beta_{ext,440nm}$, $\beta_{ext,500nm}$, $\beta_{ext,550nm}$, $\beta_{ext,670nm}$, and $\beta_{ext,870nm}$ are extinction coefficients of the entire mixture at wavelengths 440, 500, 550, 670 and 870 nm, respectively. The rest of the new output parameters are component and size specific (as above) contributions to these total extinction coefficients, i.e., the contribution by added BC (bc), OM (om), and sulfate (su) as sulfuric acid and ammonium sulfate. The contribution from ammonium sulfate, which is from cloud processing, is however zero for $k = 1 - 3$. Note that the component specific extinction coefficients in general are contributions from internally mixed components which have been added (by some production pathway) onto to background aerosol (bg). This means, for ecxample, that the total sulfate extinction coefficient (as calculated in OsloAero) is the sum of $\beta_{ext,550nm}^{su}$ and the sulfate *volume* fraction of the background extinction coefficient $\beta_{ext,550nm}^{bg}$ (see pmxsub.F90 in the OsloAero code).

The structure of aerocomk$k$.out for $k = 2 - 10$ is as for $k = 1$, except that the input variables differ in number and nature in the same way as for the kcomp$k$.out LUT files (minus the wavelength band number $iband$ which is not needed here).

The content and structure of the aerodryk$k$.out files for size-integrated information about the dry aerosol mixtures is as follows. In aerodryk*0*.out the stored information below the header is on the form

$kcomp$, C^{bg}, $C_{d<1}^{bg}$, $C_{d>2.5}^{bg}$, $A_{d<1}$, $A_{d>1}$, $V_{d<1}$, $V_{d>1}$

Here C^{bg}, $C_{d<1}^{bg}$ and $C_{d>2.5}^{bg}$ are the mass concentrations (unit $\mu g\ m^{-3}$) of the background particles for the normalized size distribution (Eq. 1) for all particle

sizes, for particles with $d < 1\mu m$ (for PM1 calculations) and $d > 2.5\mu m$ (for PM2.5 calculations, obtained from $C^{bg} - C^{bg}_{d>2.5}$), respectively. $A_{d<1}$ and $A_{d>1}$ are size-integrated dry aerosol surface areas for particles with $d < 1\mu m$ and $d > 1\mu m$, respectively, while $V_{d<1}$ and $V_{d>1}$ are the respective size-integrated dry aerosol volumes. These are in OsloAero used to calculate effective sizes, defined as $3\ V_{sizerange}/A_{sizerange}$ (unit μm) for the size ranges $d < 1\mu m$, $d > 1\mu m$, and $0.002 < d < 40\mu m$ (i.e., the whole population).

In aerodryk1.out the stored information below the header is instead on the form

$kcomp$, $fombg$, $catot$, fac, C^{bg}, $C^{bg}_{d<1}$, $C^{bg}_{d>2.5}$, C^{bc}, $C^{bc}_{d<1}$, $C^{bc}_{d>2.5}$,

C^{om}, $C^{om}_{d<1}$, $C^{om}_{d>2.5}$, C^{sc}, $C^{sc}_{d<1}$, $C^{sc}_{d>2.5}$, C^{sa}, $C^{sa}_{d<1}$, $C^{sa}_{d>2.5}$,

$A_{d<1}$, $A_{d>1}$, $V_{d<1}$, $V_{d>1}$

The new output parameters here are component (and size) specific concentrations for internally mixed (added onto the background) BC (bc), OM (om), sulfuric acid (sc, i.e., sulfate from condensation or coagulation), and ammonium sulfate (sa, from cloud processing, which is zero for $k = 1 - 3$).

In aerodryk$k$.out, where $k = 2 - 10$, the output parameters are the same as in aerodryk*1*.out, while the input variables differ in number and nature in the same way as for the aerocomk$k$.out LUT files, except that the relative humidity rh is not needed in aerodryk$k$.out.

6 Additional output for testing and case studies

Code for extra output can of course at any time be added by the user. Some often needed write statements of selected output for testing and plotting purposes are already available and can be activated by use of the last configuration option (extradiag=.true.) in section 4. These come as .dat files to separate them from the .out LUT files. LUT files and files for extra diagnostics are now also moved to separate folders after completion, to the directories LUT-output and Extra-output, respectively.

The first set of additional output which is produced are the nkcomp$k$.dat files (nkcomp$k$.out in older AeroTab versions). These files contain the modified number size distributions (Eq. 1) as function of radius r which in AeroTab ranges from ca. 0.001 - 20 μm (44 size bins). This particular output is useful for checking whether the size distributions look reasonable or not. To facilitate a direct idenifying link to the entries of the respective LUT files, the necessary (for number size distributions) input parameter values are listed after the radius and number distribution, so that all the nkcomp$k$.dat data are one the form

r(i), dndlrkny(i), cat, fac, fabc, faq, rh, kcomp

where $r(i)$ is the radius for bin number i of the sectional distribution.

The remaining .dat files do not include these production tagged input parameters. They are mainly meant for plotting purposes for cases with selected sets of input parameters, and are on a form which is easy to import and use in xmgrace (as are also the above nkcomp$k$.dat files).

The first three are the number size distributions $dN/dlogr$ before and after growth, including hygroscopic swelling, as well as the volume size distribution after growth. These files are named dndlogr0.dat, dndlogrmod.dat and dvdlogrmod.dat, respectively, and are on the form

r(i), dndlrk0(i)

r(i), dndlrkny(i)

r(i), dndlrkny(i)*(4.0*pi/3.0)*r(i)**3

The radius dependent dry volume fractions for aerosol components (and mixtures for two of the background modes) are written to the files vsi.dat, vbci.dat, voci.dat, and vai.dat. These four files are on the form

r(i), vsi(i)

r(i), vbci(i)

r(i), voci(i)

r(i), vai(i)

where *vsi* is the volume fraction of internally mixed (added onto the background) sulfate in the form of sulfuric acid or ammonium sulfate, *vbci* is the respective volume fraction of BC, *voci* that for OM, while *vai* is the volume fraction of the background component. Depending on which mixture we are looking at, the background component may consist of sulfate, OM, BC, DU (dust) or SS (sea-salt), or an internal mixture of sulfate and OM (for $k = 1$) or OM and BC (for $k = 4$). The sum of all the dry volume fractions equals 1 at all radii.

The respective radius dependent humidified volume fractions are written to the files vsol.dat, vbcsol.dat, vocsol.dat, vasol.dat and vw.dat. These five files are on the form

r(i), vssol(i)

r(i), vbcsol(i)

r(i), vocsol(i)

r(i), vasol(i)

r(i), vw(i)

where vw is the volume fraction of internally mixed water from hygroscopic swelling, and $vssol, vbcsol, vocsol$ and $vasol$ are the parameters corresponding to $vsi, vbci, voci$ and vai for the humidified particles. The sum of all the humidified volume fractions equals 1 at all radii.

Extra output of optical parameters are written to the files omega.dat, gass.dat, bext.dat, kext.dat, and mec.dat. These are on the form

xlam(iband), omega(iband)

xlam(iband), gass(iband)

xlam(iband), bext(iband)

xlam(iband), kext(iband)

xlam(iband), kext(iband)*Ctot/Cdry

where xlam is the mid-band wavelength λ, omega is SSA, gass is g, bext is β_{ext}, kext is k_{ext}, and kext*Ctot/Cdry is the traditional MEC, see Section 5.

By default, some log-info is written to the file runlog.dat during the simulation, e.g. to inform the user about how far into the multiple do loops AeroTab has come, and where it was when it failed if it crashes. Much the same info is shown on-screen. For example, for the case $kcomp = 1$, the following is written to runlog.dat:

'kcomp, irelh, ifombg, ictote, ifac=', kcomp, irelh, ifombg, ictote, ifac

There are additional print statements which are meant for control purposes, to enable the user to inspect how well the particle number and mass is conserved:

'Ntot integrated / Ntot in =', nt / ntot

'Ctot integrated / Ctot in =',
(cintbc + cintoc + cintsc + cintsa + cintbg) / (Ctot0 + Caso4 + Cabc + Caoc)

Here nt and $ntot$ are the total particle number concentrations before and after growth, which for our normalized distribution both should be 1 cm^{-3}. Furthermore, $Ctot0$ is the dry background mass concentration, $Caso4$, $Cabc$ and $Caoc$ are the total mass concentrations for added internally mixed sulfate, BC and OM before growth (as input to AeroTab), while $cintbg$, $cintsc$ and $cintsa$, $cintoc$ and $cintbc$ are the respective concentrations after growth, calculated by integrating the radius dependent mass concentrations (for the modified size distribution) over all radii. Also here the sulfate mass concentration is split in two

terms: sulfuric acid from condensation and coagulation, *cintsc*, and ammonium sulfate from cloud processing (via wet phase chemistry), *cintsa*.

7 When and how to modify AeroTab

As a first rule of thumb, whenever some of the arrays in commondefinitions.F90 need to be changed, AeroTab has to be re-run to produce new LUT. If the change only concerns background components such as mineral dust and sea-salt, then LUT only for mixtures corresponding to those components have to be remade, i.e. for $k = 6 - 7$ (dust) or $k = 8 - 10$ (sea-salt).

More generally, AeroTab needs to be updated and new LUT made whenever a new aerosol mixture is added or an existing mixture is changed with respect to complexity (e.g. by adding new components and/or new production pathways), size at the point of emission or production (R_k and/or σ_k), how much the particles are allowed to grow (as an upper threshold value for the mixture), or when the refractive index, mass density or hygroscopic properties (a product of several variables in commondefinitions.F90) of one or more of its components are changed.

Also if the structure or the format of the LUT files is changed, for instance in order to simplify the use of the AeroTab light version of the LUT in OsloAero, new LUT files have to be produced and the OsloAero code has to be modified accordingly. In the following subsections, some examples of possible modifications will be listed, along with comments on which parts of AeroTab and the corresponding OsloAero code that should be modified when changes in the aerosol scheme are made. This list should not be considered as complete, however.

7.1 Modifications which are only confined to AeroTab

Some AeroTab modifications (which change the LUT files) do not require any corresponding change in OsloAero or NorESM, apart from making sure that the new LUT are actually being read in and used, which is done on name-list level (by editing user_nl_cam).

This is for instance the case for any modifications to a component's refractive index. If there are changes in assumed hygroscopicity in the hysteresis regime (for instance linearly increasing with RH instead of the treatment described in Kirkevåg et al., 2018), which do not require changes in commondefinitions.F90, these are also confined to AeroTab.

7.2 Modifications which also require changes in OsloAero

Most modifications to AeroTab also require changes in OsloAero (NorESM2) code, either in the life-cycling code or in the code which reads in the LUT or deals with table look-ups and interpolations. As for the modifications in Section 7.1, the path to the new LUT always has to be updated.

If any of the modal parameters (R_k and σ_k) for the lognormal size distribution at the point of emission or production is to be changed, this can be done in the commondefinitions.F90 files of both AeroTab and OsloAero. Note then that also the corresponding modal parameters for aerosol life-cycling (lifeCycleNumberMedianRadius and lifeCycleSigma) in aerosoldef.F90 of OsloAero *might* need to be updated accordingly. These are assumed to have a prescribed constant growth included, and changes to these should be considered whenever R_k and/or σ_k in commondefinitions.F90 are updated. Ideally the assumed modal parameters for use in the life-cycling part of OsloAero should be replaced by values from the logntilp*k*.out LUT, with some simplified hygroscopic growth taken into account, but this potentially important link has so far not been prioritized (If you are a Master level or PhD student in search for aerosol related tasks and plan to use NorESM2, this may be a subject well worth looking into).

If the mass density or any other intensive property of one or more of the components in commondefinitions.F90 is changed, on the other hand, the only necessary changes in OsloAero are the corresponding modification in commondefinitions.F90 there.

How much a mixture can grow by internal mixing of sulfate, OM and BC onto the background component(s) and size distribution, is in AeroTab defined through the *catot* and *catote* arrays in modepar.f. Such modifications to modepar.f must be followed up by corresponding changes in *cat* and *cate* in the OsloAero code file opttab.F90. From there these arrays are made publicly available to the rest of the OsloAero code. This is also the case if changes are made to other arrays in modepar.f (such as *relh*): the corresponding array in opttab.F90 must then be modified accordingly before using the new LUT in NorESM.

Adding a new mixture is among the more complicated modifications one can do. Since arrays are not defined dynamically, the easiest way is to use the slot left available by the now obsolete $kcomp = 3$, which used to serve as a fine OM mixture just like $kcomp = 2$ does for BC, or to add code for internal mixtures also for $kcomp > 10$. If the new feature means re-introducing the OM mixture that was once used, much of the coding in AeroTab is already done, and all that is needed (with some luck) is to check if it works as expected. This has not been tested in any recent AeroTab version. The same goes for the corresponding changes in OsloAero, where old code is still present as commented lines, *often* starting with "!-3" (see pmxsub.F90).

If the change means adding an entirely new mixture, but with production pathways (condensation, coagulation and cloud processing) and complexity (number of independent input variables) already found in other existing mixtures, one can make use of the code for the existing mixture as a template, both in AeroTab and OsloAero. Introducing a new mixture with a new degree of complexity is not very different from increasing the complexity of already existing mixtures, as it may involve extensive changes to both AeroTab and OsloAero. Given that the nature of such a code extension is not known in advance, I will here only try to point to which parts of AeroTab and OsloAero that may need to be modified.

A change in number of internal mixtures or their complexity will necessarily

have to be reflected in the multiple do loop structure in AeroTab, and in the structure of the look-up tables. How to modify the various subroutines and modules of AeroTab depends on the nature of the change, but typically the following files will most probably need to be updated: AeroTab.f (new loop structure), commondefinitions.F90 (new or changed component properties), constsize.f (new process relevant constants), modepar.f (mixture properties, including growth), tabrefind.f (component refactive indices), hygro.f (component hygroscopicity), openfiles.f (if new LUT files should be added), tableinfo.f (new LUT header info), conteq.f / conteqlight.f (central in defining the mixture complexity based on production pathway), rhsub.f / rhsublight.f, koehler.f and mixsub.f (if adding new components), modetilp.f (for changed structure of the logntilp$k$.out LUT files), sizemie.f amd refind.f (for impacts of new components/mixtures on refractive indices). In short, most of the code files are involved.

The respective code files in OlsoAero which most probably need to be updated for the latter type of AeroTab changes are: opttab.F90 (reads in the kcomp$k$.out LUT files and defines the arrays for input values for all LUT), opttab_lw.F90 (reads in lwkcomp$k$.out), initaeropt.F90 (reads in aerocomk$k$.out) together with aerocopt.h and aerocop2.h, initdryp.F90 (reads in aerodryk$k$.out) together with aerodry.h, initlogn.F90 (reads in logntilp$k$.out), optinterpol.F90 (table look-ups and interpolations for kcomp$k$.out and lwkcomp$k$.out), intaeropt0.F90, intaeropt1.F90, intaeropt2to3.F90 and intaeropt5to10.F90 (table look-ups and interpolations for aerocomk$k$.out), and intlog1to3.F90, intlog4.F90 and intlog5to10.F90 (table look-ups and interpolations for logntilp$k$.out). In addition, the following code files are instrumental for the different parts of OsloAero: modalapp2.F90 (module for apportionment of internally mixed mass between mixtures), pmxsub.F90 (module where all gross aerosol optics calculations are made), parmix_progncdnc.F90 (module for calculations of aerosol sizes with respect to cloud droplet activation) and ndrop.F90 (module for droplet activation).

It is worth mentioning that some code extensions may be simplified by assuming that a new component has approximately the same properties as an already existing component. This is the case for the ongoing work on a NorESM2 version with more complex chemistry and with the additional aerosol component nitrate. Since there is little information available about the hygroscopic and optical properties of nitrate aerosols, and since it is computationally expensive (prohibitive) to add to the maximum number of dimensions (input parameters) of the LUT, we will for this model version assume that the nitrate aerosol has the same refractive index as function of wavelength and the same hygroscopicity as that of either sulfuric acid or ammonium sulfate, or that the properties of one of these two components apply for both sulfate and nitrate in general, in order to simplify even more.

One final example is one where the spectral bands have to be changed as a result of changes in the radiative transfer scheme in NorESM. This was the case when going from NorESM1 to NorESM1.2 / NorESM2, due to an upgrade from CAMRT to RRTMG in the host model CESM. If such a change is required again, at some point, AeroTab must be modified to take the number and the boundaries of the new spectral bands into account in a similar way as done back

then. The code modifications in AeroTab from that time can therefore be used as a "template", e.g. by comparing the sections of the code which are active when $ib = 29$ vs. $ib = 31$. In OsloAero the change must similarly be reflected in the number of wavelength bands in all aerosol optics calculations (reading in the LUT, look-ups and interpolations), and possibly also the ordering of bands (in pmxsub.F90) for use in the radiation code (radiation.F90).

7.3 OsloAero changes which do not involve AeroTab

Most changes to OsloAero do not involve AeroTab. Typically this is true for any modification which does not concern the intensive properties of the aerosols (as particle populations) treated in OsloAero. A few examples: new emission inventories or interactive emission flux formulations (unless particle sizes at the point of emission need to be updated), changes in prescribed below-cloud scavenging efficiencies or in coating assumptions (not treated in AeroTab) with respect to activation and in-cloud scavenging, assumptions about convective mixing, clear-sky optics assumptions, etc.

7.4 Suggestions for future improvements of AeroTab

The first version of AeroTab was made at a time where updates of the intensive properties of aerosols for use in a climate model were made less frequently than is the case today. The number of NorESM users and projects this model is applied in has increased manyfold since then, and new types of modelling activities have arisen, such as the AeroCom multi-model perturbed parameter ensemble experiments (see https://wiki.met.no/aerocom/phase3-experiments), which require a high degree of flexibility and speed with respect to making changes in the aerosol micro-physics code.

Some modifications which may improve AeroTab and make it better equipped for present and future challenges have already been mentioned, like the restructuring and simplification of LUT produced with AeroTab light (if the accuracy of this method is deemed acceptable), which must be followed by corresponding changes in OsloAero in order to make also NorESM more CPU efficient.

In the earliest versions of AeroTab, the weakest link CPU-wise was the Mie code and the calculations of aerosol growth. When calculations of LUT for CCN as function of (prescribed) super-saturation were replaced with LUT for the size parameters of the lognormally fitted size distributions (used as input to the cloud droplet activation code in all published versions of NorESM), this part of the code became the overall slowest when run in its standard configuration (i.e., not the AeroTab light version). The method for solving the least squares problem in this part of the code should therefore probably be reviewed and, if feasible, improved.

Another suggestion is to restructure the whole code to enable changes in the scheme with fewer manual code changes (to enhance its ease of use), and to enable AeroTab to run all LUT in one operation, at least as a configuration option. The simplest approach for the latter objective is to make a new main

program which loops over the various configuration options and calls AeroTab as a sub-routine, with the configuration options as input values. A better approach in the long run, which also addresses the first objective, is to rewrite AeroTab to use global arrays to a much larger extent.

The code should also be modified to facilitate simulations on multiple nodes. So far AeroTab has only been run in "manually parallelized" mode, i.e., by producing different sets of LUT in different sessions (windows) or on different machines at the same time.

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