UI Aerosol Hygroscopicity and Mixing State Package

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Contents

1 Theoretical base

1.1 Convert Aerosol Mass Concentration to Aerosol Optical Thickness

The definition of the aerosol optical depth (AOD) is the integration of the aerosol extinction coefficient over a certain optical path given by,

$$\tau(s_1, s_2) = \int_{s_1}^{s_2} \beta_e(s) ds \tag{1}$$

where s is the distance of the optical path.

For particle that has a radius of r and density of ρ in a volume of air, the number of the particle can be calculated by,

$$N = \frac{C}{\rho v} = \frac{3C}{4\pi r^3 \rho} \tag{2}$$

where C is the mass concentration, $v = \frac{4}{3}\pi r^3$. consequently, the extinction coefficient of the particle is given by,

$$\beta_e = N\pi r^2 Q_{ext} \tag{3}$$

where Q_{ext} is the extinction efficiency. Thus,

$$\tau(s_1, s_2) = \int_{s_1}^{s_2} \frac{3Q_{ext}C}{4r\rho} ds \tag{4}$$

1.2 Aerosol with size distribution

For aerosol that obeys a size distribution $n(r)$, following the deduction above and assume the average number of particle is N_a, then the extinction coefficient is given by,

$$\begin{aligned} \beta_e &= \frac{CN_a}{\rho \int_0^\infty \frac{4}{3}\pi r^3 n(r) dr} \frac{\int_0^\infty \pi r^2 n(r) Q_{ext} dr}{N_a} \\ &= \frac{CN_a \int_0^\infty \frac{4}{3}\pi r^2 n(r) dr}{\rho \int_0^\infty \frac{4}{3}\pi r^3 n(r) dr} \frac{\int_0^\infty \pi r^2 n(r) Q_{ext} dr}{N_a \int_0^\infty \frac{4}{3}\pi r^2 n(r) dr} \\ &= \frac{3C\tilde{Q}_{ext}}{4\rho r_e} \end{aligned} \tag{5}$$

where r_e is defined as the effective radius of the particles that has a size distribution of $n(r)$ given by,

$$r_e = \frac{\int_0^\infty \pi r^3 n(r) dr}{\int_0^\infty \pi r^2 n(r) dr} \tag{6}$$

$\tilde{Q}_{ext}$ is the uses an area weighted extinction efficiency given by,

$$\tilde{Q}_{ext} = \frac{\int_0^\infty \pi r^2 n(r) Q_{ext} dr}{\int_0^\infty \pi r^2 n(r) dr} \tag{7}$$

To be continue...

2 Getting Start

2.1 Directory Structure Overview

A short description of each sub-directory for the hygroscopicity and mixing state package:

- src/: Folder to carry several uncompiled source codes.
- run/: Run folder used to run the model, which contains necessary namelist file and input files.
- data/: Data folder to support the running of the model

2.2 Compile hygroscopicity and mixing state package

A full compilation is necessary when you first get the codes. It could be done by executing the file makefile in the src foder, which will compile hygroscopicity and mixing state package and all of the necessary libraries.

2.3 Run

To run the model, just move/copy the generated executable file hygroscopic.exe upon compilation to the run directory, and run it with the specification of the input file namelist.ini.

3 Mandatory input file: namelist.ini

3.1 The CONTROL Menu

```
%%% CONTROL MENU %%%     :
Run     directory         : .../hygroscopic/modulized
Data    directory         : .../hygroscopic/data
Output  directory         : .../hygroscopic/modulized
```

Description:

1. Title for this menu.
2. Specifies the model run directory. Generally, it is "./" which indicates the current directory
3. Specifies the directory where the ancillary data is placed.
4. Specifies the subdirectory where the model output will be saved.

3.2 The Radiation Menu

```
%%% RADIATION MENU %%%  :
Wavenumber as input?     : F
Spectra set (nm or 1/cm): 670
  - interval(nm or 1/cm): 5
Relative Humidy          : 0 20 40 50 52.5 55 57.5
```

Description:

1. Title for this menu.
2. Switch to turn on/off the frequency as spectral input for the following three lines: A "T" is for frequency-mode input in the units of cm^{-1} ; An 'F' is for wavelength input in the units of nanometer (nm). current directory
3. Specifies the spectral range in the units of nanometer or cm^{-1} . User can specify either a single spectrum or multiple spectra. It should be noted that, for multiple spectrum, the input values should be in an ascending sequence..
4. Specifies the relative humidy in %

3.3 The Aerosol Menu

```
%%% AEROSOL MENU %%%     :
External Mix?             : T
Internal Mix?             : T
BC/Sulfate Mass Ratio     : 0.05
Dust/All Mass Ratio       : 0
Sulfate #1 Properties     :
     ........................................
  - species ID            : 1 2 3 4 5 6
  - species mass ratio    : 1 0 0 0 0 0
  - size range [um]       : 0.005      20.0
  - size distribution     : PAR(1)     PAR(2)
            ==> Entries   : 0.07         1.8
BC   #1 Properties        :
     ........................................
  - density               : 1.0
  - refractive index      : 1.76       0.46
  - size range [um]       : 0.005      20.0
  - size distribution     : PAR(1)     PAR(2)
            ==> Entries   : 0.0118     1.8
Dust #3 Properties        :
     ........................................
```

```
19 ||  - density                : 2.0
20 ||  - refractive index      : 1.53        0.008
21 ||  - size range [um]       : 0.001       60.0
22 ||  - size distribution     : PAR(1)      PAR(2)
23 ||            ==> Entries  : 0.47        2.50
```

Description:

1. Title for this menu.
2. Switch to turn on/off the external mixing calculation.
3. Switch to turn on/off the internal mixing calculation
4. Specifies mass ratio for the black carbon to sulfate in decimal.
5. Specifies mass ratio for the dust to (BC + sulfate) in decimal.
6. Title for Sulfate.
7. specify the sulfates:
   1 Ammonium sulfate, $(NH_4)_2SO_4$
   2 Ammonium bisulfate, NH_4HSO_4
   3 $(NH_4)_3H(SO_4)_2$
   4 NaCL
   5 NH_4NO_2
   6 H_2SO_4
8. Specify the mass ratio of each sulfate selected above
9. Particle size range in micron-meter.
10. Size distribution entries titles (lognormal size distribution).
11. Specify PAR(1) as the R_g and PAR(2) as the σ_g of lognormal size distribution.
12. Title for BC.
13. Specify the density of BC.
14. Refractive index for BC, respectively, real and imaginary terms.
15. Particle size range in micron-meter.
16. Size distribution entries titles (lognormal size distribution).
17. Specify PAR(1) as the R_g and PAR(2) as the σ_g of lognormal size distribution.
18. Title for dust.
19. Specify the density of dust.
20. Refractive index for dust, respectively, real and imaginary terms.
21. Particle size range in micron-meter.
22. Size distribution entries titles (lognormal size distribution).
23. Specify PAR(1) as the R_g and PAR(2) as the σ_g of lognormal size distribution, respectively.

3.4 The Diagnostic Menu

```
%%% DIAGNOSTIC MENU %%% :
Turn on DIAGNOSTIC        : F
Output NC file prefix     : test
```

Description:

1. Title for this menu.
2. Switch to turn on/off of generating the diagnostic file.
3. Specifies a prefix name for the diagnostic file (netCDF format).

4 Output Files

The variables saved to the netCDF files are controlled by the Diagnostic Menu in namelist.ini for different categories. Here we list those variables in below Table 3.2–3.10. The netCDF file also contains a few global atrributes (Table 3.1) that could be helpful for quick and generic check on the simulation.

Table 1: Table 3.1: List of global attributes of the diagnostic netCDF file

Attribute	Value	Description
Title	File Name	H & M Diagnostic File
History	Time	Time of the .nc file is created
Model	Hygroscopicity & Mixing	Mode name
Version	x.x.x	Model version number
Enternal	On/Of	If including enternal mixing?
Internal	On/Of	If including internal mixing?
Success	Yes/No	If simulation is successful?

Table 2: Table 3.2: List of dimensions

Attribute	Value	Description
Spectra	NSPECTRA	Number of spectrum
RH	NRH_LST	Number of relative humidity
Sulfate	NSULF	Number of sulfate in total
SulfMass.	NSULFMASSRATIO	Number of sulfate used
BcMRatio	NBC2SULF_MASS	Number of BC to sulfate mass ratio
Angle	NANG	Number of dust to (BC + sulfate mass) ratio

Table 3: Table 3.3: List of Variables

Variable	Units	Longname
LAMDAS	nm	Spectral wavength
Wavenum	cm^-1	Spectral frequency
RH	none	Relative Humidity
SulfMassRatio	none	Sulfate mass ratio
BcMassRatio	none	BC to sulfate mass ratio
DustMassRatio	none	Dust to all mass ratio
DisPara	none	Species size distribution
SulfNames	none	Sulfate species names
SulfDryV	none	Sulfate dry volume
SulfDryMass	none	Sulfate dry mass
SulfDryRho	none	Sulfate dry density
SulfWetV	none	Sulfate wet volume
SulfWetMass	none	Sulfate wet mass
SulfWetRho	none	Sulfate wet density
SulfAvgGF	none	Sulfate growth factor
SulfAvgMGF	none	Sulfate mass growth factor
BcRho	g/cm^3	BC density
BcMR	none	BC Real-part refractive index
BcMI	none	BC Imaginary-part refractive index
BcREFF	um	BC Effective radius
BcVEFF	um	BC Effective variance

BcAREA	um^2	BC Surface area
BcVOLUME	um^3	BC Volume
DustRho	g/cm^3	Dust density
DustMR	none	Dust Real-part refractive index
DustMI	none	Dust Imaginary-part refractive index
DustREFF	um	Dust Effective radius
DustVEFF	um	Dust Effective variance
DustAREA	um^2	Dust Surface area
DustVOLUME	um^3	Dust Volume - dust
WaterMr	none	Water refractive index
SulfCompMR	none	Sulfate composite Real-part refractive
SulfSpecMR	none	Sulfate species Real-part refractive ind
SANGLE	none	Scattering angle
BcTotalV	none	BC total volume
SulfBcRRATIO	none	Sulf to BC radius ratio
SulfBcGF	none	Sulf-BC growth factor
SulfBcMGF	none	Sulf-BC mass growth factor
SulfBcRHO	g/cm^3	Sulf-BC density
BcSSA	none	BC Single scattering albedo
BcASY	none	BC Asymmetric factor
BcCEXT	none	BC Extinction cross section
BcCSCA	none	BC Scattering cross section
BcEXTEFFCY	none	BC Extinction coefficient
BcMEXTEFFCY	none	BC Mass extinction coefficient
BcHBSCAT	none	BC Hemispheric backscattering
BcEXTTOBCARATIO	none	BC Extinction to back scattering ratio
BcPHASE	none	BC Phase function
DustSSA	none	Dust Single scattering albedo
DustASY	none	Dust Asymmetric factor
DustCEXT	none	Dust Extinction cross section
DustCSCA	none	Dust Scattering cross section
DustEXTEFFCY	none	Dust Extinction coefficient
DustMEXTEFFCY	none	Dust Mass extinction coefficient
DustHBSCAT	none	Dust Hemispheric backscattering
DustEXTTOBCARATIO	none	Dust Extinction to back scattering ratio
DustPHASE	none	Dust Phase function
SulfCompREFF	um	Sulfate composite Effective radius
SulfCompVEFF	um	Sulfate composite Effective variance
SulfCompAREA	um^2	Sulfate composite Surface area
SulfCompVOLUME	um^3	Sulfate composite Volume
SulfCompSSA	none	Sulfate composite Single scattering albe
SulfCompASY	none	Sulfate composite Asymmetric factor
SulfCompCEXT	none	Sulfate composite Extinction cross secti
SulfCompCSCA	none	Sulfate composite Scattering cross secti
SulfCompEXTEFFCY	none	Sulfate composite Extinction coefficient
SulfCompMEXTEFFCY	none	Sulfate composite Mass extinction coeffi
SulfCompHBSCAT	none	Sulfate composite Hemispheric backscatte
SulfCompEXTTOBCARATIO	none	Sulfate composite Extinction to back sca
SulfCompPHASE	none	Sulfate composite Phase function

ExMixCEXT	none	External mixing Extinction cross section
ExMixSSA	none	External mixing Single scattering albedo
ExMixREFF	um	External mixing Effective radius
ExMixNUM	none	External mixing Total Number
ExMixPHASE	none	External mixing Phase Function
InMixCEXT	none	Internal mixing Extinction cross section
InMixSSA	none	Internal mixing Single scattering albedo
InMixREFF	um	Internal mixing Effective radius
InMixNUM	none	Internal mixing Total Number
InMixPHASE	none	Internal mixing Phase Function