MOPSMAP v1.0 user guide

'Modelled optical properties of ensembles of aerosol particles'

https://mopsmap.net

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Contents

1 General description

MOPSMAP is a tool for modeling optical properties of ensembles of aerosol particles. It consists of a single particle data set, a Fortran program performing the actual calculations, and a web interface providing interactive access to the program. The data set contains the optical properties of single particles (or narrow size bins) on a grid of sizes, shapes, and refractive indices. These optical properties are interpolated and superimposed by the Fortran program to calculate optical properties of user-defined particle mixtures. A general description of MOPSMAP is given in a GMD paper at https://www.geosci-model-dev-discuss.net/gmd-2018-56/. The data set and the Fortran program for offline calculations are available for download at https://doi.org/10.5281/zenodo.1284217. The web-interface for online calculations is provided at https://mopsmap.net. This user guide is available online under https://mopsmap.net/mopsmap_userguide.pdf.

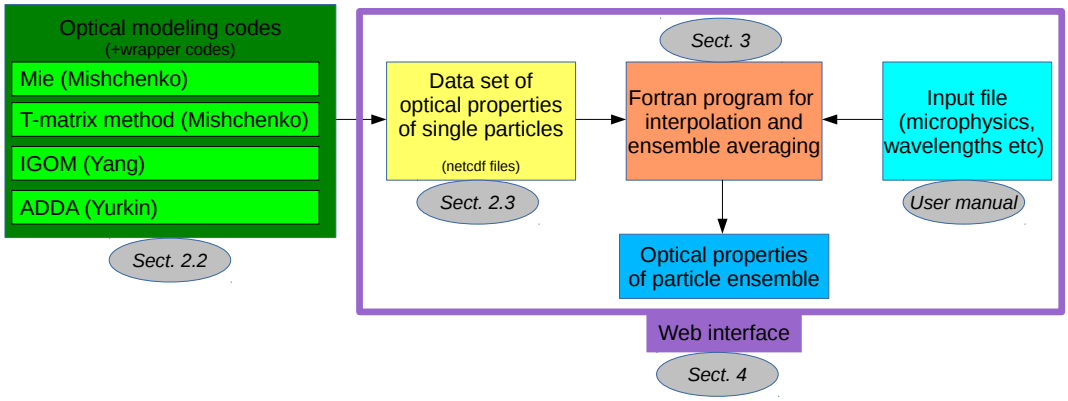

Figure 1: *General overview of MOPSMAP. This user guide mainly describes how to use the Fortran program including its input and output.*

This user guide mainly describes how to use the Fortran program, how to set up the input file, and how to interpret its output. It is also required for users of the expert mode of the MOPSMAP web-interface where the input file of the Fortran program can be modified individually. This user guide in not required for those using the normal mode of the web-interface but still might be helpful for understanding. Comments about the availabilty of options in the web interface are given below (in grey font).

If a command line argument is given for starting the Fortran program, the argument is interpreted as the name of the input file. If no command line argument is given, `input_mopsmap.txt` is assumed as the name of the input file.

2 Input file

The input file specifies the microphysics of the aerosol ensemble and the wavelengths to be calculated, as well as the output options. The microphysical properties of the aerosol ensembles modelled by MOPSMAP are described by 'modes' (or equivalently 'components'). Each mode is characterized by a particle size (distribution), a particle shape (distribution), and a refractive index. An ensemble consists of at least one mode. The input options are read line-by-line from the input file and described in this section.

The input file consists of lines having the following structure:

[**prefix**] **keyword** [**specifier**] [*argument1 argument2 argument3* ...].

These colors are used in the following to facilitate the reading, optional values are included in square brackets.

The prefix is optional and required if the keyword shall address only one specific mode ("aerosol component") i (with i being the number of the mode), otherwise all modes are addressed. The prefix can only be mode 1, mode 2, etc. according to the number of the mode that should be addressed. The number of modes is not limited by the code. The total number of modes used in the calculations is determined by the maximum mode i_{max} addressed by a prefix in the input file. If nowhere in the input file a prefix is given, a monomodal ensemble is assumed (i_{max}=1). For all modes from 1 to i_{max} the keywords size, shape, and refrac need to be specified in the input file. If the specifier and the arguments of the keyword are the same for all modes it is recommended to use the keyword without prefix.

- Example: Ensemble with three modes having different properties of keyword1:

  mode 1 keyword1 specifier1 *argument11 argument21*
  mode 2 keyword1 specifier2 *argument12 argument22*
  mode 3 keyword1 specifier3 *argument13 argument23*

- Example: Ensemble with three modes having the same properties of keyword1:

  mode 1 keyword1 specifier1 *argument11 argument21*
  mode 2 keyword1 specifier1 *argument11 argument21*
  mode 3 keyword1 specifier1 *argument11 argument21*

  equivalent to:

  keyword1 specifier1 *argument11 argument21*

- Example: Ensemble with two out of three modes having the same properties of keyword1:

  mode 1 keyword1 specifier1 *argument11 argument21*
  mode 2 keyword1 specifier1 *argument11 argument21*
  mode 3 keyword1 specifier2 *argument12 argument22*

equivalent to:

keyword1 specifier1 *argument11 argument21*
mode 3 keyword1 specifier2 *argument12 argument22*

The following keywords are available:

- Mandatory keywords with optional prefix are:

$$\text{keyword} = \begin{cases} \text{size} \\ \text{shape} \\ \text{refrac} \end{cases}$$

- Optional keywords with optional prefix:

$$\text{keyword} = \begin{cases} \text{density} \\ \text{kappa} \end{cases}$$

- Mandatory keywords without prefix:

$$\text{keyword} = \begin{cases} \text{output} \\ \text{wavelength} \end{cases}$$

- Optional keywords without prefix:

$$\text{keyword} = \begin{cases} \text{rH} \\ \text{water\_refrac\_file} \\ \text{size\_equ} \\ \text{diameter} \\ \text{scatlib} \\ \text{status} \\ \text{debug} \end{cases}$$

Any other keyword results in an error message.

The order of the lines in the file is not relevant except when the same combination of prefix and keyword is used repeatedly. In that case only the last occurrence is considered.

Lines starting with # are considered as comments.

Any filename specified in the input file (for refractive index, etc.) should be in quotation marks. Otherwise MOPSMAP might not be able to read the path properly.

2.1 Keywords with optional prefix, describing the aerosol microphysics

As mentioned the keyword is applied to the specified mode if a prefix is given, and it is applied to all modes if no prefix is given.

2.1.1 Keyword: size

All sizes need to be given in μm for correct calculation of extensive properties. This keyword can have one of the following specifiers.

$$\text{specifier} = \begin{cases} none \\ \text{distr\_list} \\ \text{distr\_file} \\ \text{bin\_file} \\ \text{log\_normal} \\ \text{mod\_gamma} \end{cases}$$

Depending on the specifier, different arguments are required.

- [**mode i**] **size** r n_0

  Defines the radius r of a single particle (given in μm).

  The total particle number density n_0 needs to be given in units of m^{-3}.

  In web interface: Available in expert mode.

- [**mode i**] **size distr_list** *distr_type* r_1 n_1 r_2 n_2 r_3 n_3 ...

  Determines the size distribution on a user defined grid.

  $r_1 < r_2 < r_3 \ldots$ specify the radius grid points in ascending order (given in μm). n_1, n_2, n_3, etc. specify the size distribution values at the corresponding radius grid. The interpretation of the size distribution values depends on *distr_type*, which can take one of the following values:
  $\{dndr|dndlnr|dndlogr|dadr|dadlnr|dadlogr|dvdr|dvdlnr|dvdlogr\}$.

  The n_i values describe a concentration as particle number, cross section area, or volume per radius, ln(radius), or log(radius) interval depending on *distr_type*.

  The units of the n_i values are $m^{-3}\mu m^{-1}$ for $dndr$, m^{-3} for $dndlnr$ and $dndlogr$, $m^2m^{-3}\mu m^{-1}$ for $dadr$, m^2m^{-3} for $dadlnr$ and $dadlogr$, $m^3m^{-3}\mu m^{-1}$ for $dvdr$, and m^3m^{-3} for $dvdlnr$ and $dvdlogr$.

  The size distribution values are interpolated between the radius grid points.

  In case keyword diameter (see below) is used, the r_i values of each line are interpreted as diameter and the n_i as concentration per diameter, ln(diameter), or log(diameter) interval.

The maximum line length is limited to 990 characters.

In web interface: Available in expert mode.

- [**mode i**] **size distr_file** *distr_type distr_filename*

  Reads the size distribution from the file *distr_filename*. The interpretation of the data in *distr_filename* depends on *distr_type*, which can take one of the following values:
  $\{dndr|dndlnr|dndlogr|dadr|dadlnr|dadlogr|dvdr|dvdlnr|dvdlogr\}$.

  The file *distr_filename* contains a number of lines with two values each. The first value is the radius, given in μm. Radii must be given in ascending order. The radius integration range is from the radius in the first line to the radius in the last line. The second value describes the concentration analogous to the n_i values described above for **size distr_list**.

  In web interface: Not available.

- [**mode i**] **size bin_file** *bin_filename*

  Reads the binned size distribution from the file *bin_filename*.

  The file *bin_filename* contains a number of lines with two values each. The first value is the radius, given in μm. Radii must be given in ascending order. The second value is the number concentration (in units of m^{-3}) of particles in the radius range from the first value of the same line to the first value of the subsequent line. In the calculations constant dn/dr is assumed within each bin. A second value needs to be given in the last line, but the value is ignored.

  In web interface: Not available.

- [**mode i**] **size log_normal** r_{mod} σ n_0 r_{min} r_{max}

  Defines a log-normal size distribution (particle number density per particle radius interval) according to

$$n(r) = \frac{1}{\sqrt{2\pi}} \frac{N_0}{\ln \sigma} \frac{1}{r} \exp\left[-\frac{1}{2}\left(\frac{\ln r - \ln r_{mod}}{\ln \sigma}\right)^2\right]$$

  Particles in the radius range from r_{min} to r_{max} are covered.

  The total particle number density n_0 needs to be given in units of m^{-3}. Note that the actual particle number density of the modeled ensemble may be lower than n_0 because of clipping at r_{min} and r_{max}.

  In web interface: Available. In the normal mode of the web interface n_0 is given in units of cm^{-3}.

- [**mode i**] **size mod_gamma** a r_{min} r_{max} α b γ

  Defines a modified gamma distribution (particle number density per particle radius interval) according to

$$n(r) = Ar^{\alpha} \exp\left(-Br^{\gamma}\right)$$

Particles in the radius range from r_{min} to r_{max} are covered.

The parameter A needs to be given in units of m^{-3}.

In web interface: Available in expert mode.

2.1.2 Keyword: shape

This keyword can have one of the following specifiers.

$$\text{specifier} = \begin{cases} \text{sphere} \\ \text{spheroid} \\ \text{irregular} \\ \text{irregular\_overlay} \end{cases}$$

Depending on the specifier, different arguments are required.

- [**mode i**] **shape sphere**

  Spherical particles are assumed.

  In web interface: Available.

- [**mode i**] **shape spheroid** *ob_pro* ϵ'

  Spheroidal particles are assumed. The argument *ob_pro* can have one of the following values: $\{oblate|prolate\}$ for oblate or prolate spheroids with aspect ratio ϵ' (≥ 1) assumed.

  In web interface: Available.

- [**mode i**] **shape spheroid log_normal** ζ_1 ζ_2 ϵ'_0 σ_{ar}

  Mixture of spheres and spheroids with a modified log-normal aspect ratio distribution.

  ζ_1 is the ratio of spheroids to all particles (other particles are spheres). ζ_2 is the ratio of prolate spheroids to all spheroids. Thus, 1-ζ_1 are spheres, $\zeta_1 \times \zeta_2$ are prolate spheroids, and $\zeta_1 \times (1 - \zeta_2)$ are oblate spheroids.

  The aspect ratio distribution of the spheroids is given by:

$$f(\epsilon') = \frac{1}{\sqrt{2\pi}\sigma_{ar}(\epsilon' - 1)} \exp\left[-\frac{1}{2}\left(\frac{\ln(\epsilon' - 1) - \ln(\epsilon'_0 - 1)}{\sigma_{ar}}\right)^2\right]$$

  Aspect ratios from $1.2 \leq \epsilon' \leq 5.0$ are covered.

  In web interface: Available.

- [**mode i**] **shape spheroid distr_file** *distr_filename*

  Reads spheroid aspect ratio distribution from file *distr_filename*. The first line contains the ratio of prolate spheroids ζ. All subsequent lines contain two values: the aspect ratio ($1.0 < \epsilon' \leq 5.0$) and its relative weight. The sum of all weights is normalized to 1.

  In web interface: Two distributions are available.

- [**mode i**] **shape irregular** *shape_id*

  All particles have an irregular shape according to the identifier *shape_id* with one of the following values: $\{A|B|C|D|E|F\}$. These irregular particles are defined in Gasteiger at al. (2011).

  In web interface: Available in expert mode.

- [**mode i**] **shape irregular distr_file** *distr_filename*

  Reads irregular shape distribution from the file *distr_filename* that contains a number of lines with two values each. The first value is the identifier of the shape and the second is its relative weight. The sum of all weights is normalized to 1.

  In web interface: Not available.

- [**mode i**] **shape irregular_overlay** *distr_filename* x_{min} x_{max}

  The file *distr_filename* contains a number of lines with two values each. The first value is the identifier of the shape and the second is its relative weight. The sum of all weights is normalized to 1. These irregularly shaped particles are used in the size parameter range from x_{min} to x_{max}.

  The particle shape outside this size parameter range has to be specified with the other shape options.

  In web interface: Not available.

2.1.3 Keyword: refrac

This keyword can have one of the following specifiers.

$$\text{specifier} = \begin{cases} \textit{none} \\ \text{file} \\ \text{nonabs\_fraction} \end{cases}$$

- [**mode i**] **refrac** m_r m_i

  Assumes a wavelength-independent refractive index $m = m_r + m_i\, i$ ($m_i \geq 0$).

  In web interface: Available.

- [**mode i**] **refrac file** *refrac_filename*

  Reads refractive index from file *refrac_filename* containing a number of lines with three values each: wavelength (in μm), real part of the refractive index m_r, and

imaginary part of the refractive index m_i. The wavelengths need to be in ascending order.

In web interface: Several predefined sets available.

- [**mode i**] **refrac nonabs_fraction** χ

  Non-absorbing fraction approach: Replace an ensemble of absorbing particles ($\overline{m_i}$) with a mixture of non-absorbing and (stronger) absorbing particles. The fraction χ (with $0 < \chi < 1$) determines the relative number of non-absorbing particles (m_i=0). The imaginary part of the refractive index of the fraction (1-χ) is $m_i = \overline{m_i}/(1-\chi)$ so that the mean refractive index of the mixture is preserved.

  In web interface: Available in expert mode.

2.1.4 Keyword: density

- [**mode i**] **density** ρ

  Defines the particle density ρ in $g\,cm^{-3}$. If this keyword is missing, $\rho = 2.6\,g\,cm^{-3}$ is assumed.

  In web interface: Available.

2.1.5 Keyword: kappa

- [**mode i**] **kappa** κ

  Defines the hygroscopicity parameter κ. This keyword is mandatory if the keyword rH (see below) is used.

  In web interface: Available.

2.2 Keywords without prefix

2.2.1 Keyword: wavelength

Selection of the wavelengths of the optical properties to be calculated.

All wavelengths need to be given in μm.

In web interface: The wavelengths in the normal mode of the web interface need to be given in nanometers.

This keyword can have one of the following specifiers:

$$\text{specifier} = \begin{cases} \textit{none} \\ \text{range} \\ \text{list} \\ \text{file} \\ \text{from\_refrac\_file} \end{cases}$$

Depending on the specifier, different arguments are required.

- **wavelength** λ

  Single wavelength λ in μm.

  In web interface: Available.

- **wavelength range** λ_{min} λ_{max} λ_{step}

  Definition of an equidistant wavelength grid from λ_{min} to not larger than λ_{max} with step width λ_{step}.

  In web interface: Available.

- **wavelength list** λ_1 λ_2 ...

  List of wavelengths (μm) in ascending order. The length of the line in the input file is limited to about 990 characters.

  In web interface: Available.

- **wavelength file** *wavelength_file*

  Reads the wavelength grid from the file *wavelength_file* containing a number of lines with one wavelength in μm each. The wavelengths need to be in ascending order. The file *wavelength_file* can be the same as *refrac_filename* (see keyword/specifier refrac file); in this case only the first value in each line is considered.

  In web interface: Not available.

- **wavelength from_refrac_file**

  Uses wavelength grid from the file *refrac_filename* (see keyword/specifier refrac file) of the first mode.

  In web interface: Available in expert mode.

2.2.2 Keyword: rH

- **rH** *rel_hum*

  Sets the relative humidity to *rel_hum* (in %) in the range from 0 to 99.

  If this keyword is used, all sizes, refractive indices and densities given in the input file are interpreted as 'dry properties' and the hygroscopicity parameter κ needs to be specified. The size of 'wet properties', which are used for the optical calculations, are calculated using

$$\frac{r_{wet}(rel\_hum)}{r_{dry}} = \left(1 + \kappa \cdot \frac{rel\_hum}{100 - rel\_hum}\right)^{\frac{1}{3}}$$

  Refractive indices and densities of the wet particles are determined as weighted means from dry particles and water. The particle shape is not modified.

  If this keyword is not set, a relative humidity of 0 is assumed.

  In web interface: Available.

2.2.3 Keyword: size_equ

- **size_equ** *size_def*

  Definition of particle radius.

  The argument *size_def* can have one of the following values: $\{cs|vol|vol\_cs\_ratio\}$. If this keyword is not specified, $size\_def = cs$ is assumed.

  If *cs* is selected, all particle sizes are interpreted as cross-section-equivalent radii $r_c = \sqrt{C_{geo}/\pi}$, where C_{geo} is the orientation-averaged cross section of the particles.

  If *vol* is selected, all particle sizes are interpreted as volume-equivalent radii $r_v = \sqrt[3]{3V/(4\pi)}$, where V is the particle volume.

  If *vol_cs_ratio* is selected, all particle sizes are interpreted as radii of spheres that have the same ratio between volume and geometric cross section as the particle. For a given particle, the radius is thus defined as $r_{vol\_cs\_ratio} = 3V/(4C_{geo}) = (r_v/r_c)^3 \cdot r_c$.

  In web interface: Available.

2.2.4 Keyword: diameter

- **diameter**

  If this keyword is given, all particle 'radius' values given in the input file are interpreted as diameters.

  In web interface: Available in expert mode.

2.2.5 Keyword: water_refrac_file

- **water_refrac_file** *water_refrac_file*

  Specifies the file with the wavelength-dependent refractive index of water which is used to calculate the refractive index in case of wet particles (i.e. when $\kappa > 0$ and $rel\_hum > 0$). The file structure is the same as for refrac file, i.e. each line contains the wavelength, the real part, and the imaginary part of the refractive index. By default, *water_refrac_file* is set to '../data/refr_water_segelstein'.

  In web interface: Alternative file '../data/refr_water' available in expert mode.

2.2.6 Keyword: output

This keyword is used to define the type and format of the output. It can have one of the following specifiers:

$$\text{specifier} = \begin{cases} \text{integrated} \\ \text{phase\_function} \\ \text{scattering\_matrix} \\ \text{volume\_scattering\_function} \\ \text{lidar} \\ \text{coeff} \\ \text{digits} \\ \text{ascii\_file} \\ \text{netcdf} \\ \text{num\_theta} \\ \text{theta\_file} \\ \text{num\_coeff} \\ \text{header} \end{cases}$$

Depending on the specifier, different arguments are required.

- **output integrated**

  The output contains integrated parameters in ASCII format, for details see Sect. 3.

  In web interface: Automatically enabled.

- **output phase_function**

  The output contains the normalized phase function as function of angle in ASCII format, for details see Sect. 3.

  In web interface: Automatically enabled.

- **output scattering_matrix**

  The output contains all six elements of the scattering matrix as function of angle in ASCII format, for details see Sect. 3.

  In web interface: Automatically enabled.

- **output volume_scattering_function**

  The output contains the volume scattering function as function of angle in ASCII format, for details see Sect. 3.

  In web interface: Automatically enabled.

- **output lidar**

  The output contains lidar-relevant parameters in ASCII format, for details see Sect. 3.

  In web interface: Automatically enabled.

- **output coeff**

  The output contains the expansion coefficients of the scattering matrix in ASCII format, for details see Sect. 3.

In web interface: Available in expert mode.

- **output digits** n_{digits}

  Defines the number of significant digits in the ASCII output, n_{digits} can have values between 3 and 15 (default is 6).

  In web interface: Available in expert mode.

- **output ascii_file** *[ascii_filename]*

  Instead of printing the output to the screen (if this keyword/specifier is not given), the ASCII output is written to files as follows: For each type of output a separate file is created. Their filenames consist of the string given in *ascii_filename* and the specific extension (e.g. 'testcase01.scattering_matrix' for the scattering matrix if *ascii_filename* is 'testcase01'). If no argument *ascii_filename* is given, the name of the input file is used as basename for the output files.

  In web interface: Automatically enabled.

- **output netcdf** *nc_filename [switch]*

  Output in netcdf format is written to file *nc_filename*. The optional argument *switch* can be one of the following values: {*reff* | *hum*} (default: *reff*). It specifies whether the file contains the variable *reff* or variable *hum*. The format is such that the file can be used by the radiative transfer code uvspec included in libRadtran (see `http://libradtran.org`). An example on how to use this file with uvspec is available in the directory 'misc/libRadtran'.

  In web interface: Available.

- **output num_theta** n_θ

  Specifies the number of equidistant scattering angles n_θ in the output where applicable. If this keyword/specifier is not used, n_θ=181, i.e. $\theta = 0°, 1°, 2°, ..., 180°$.

  In web interface: Available.

- **output theta_file** *filename*

  Specifies a (arbitrary) grid of scattering angles used for the output. The file *filename* has to contain one degree value (in the range from 0° to 180°) per line in ascending order.

  In web interface: Not available.

- **output num_coeff** l_{max}

  Specifies the maximum number l_{max} of expansion coefficients in the output (relevant for specifiers coeff and netcdf).

  In web interface: Available in expert mode.

- **output header**

  If this keyword/specifier is used a header explaining the content of the output-values is added to all output files.

  In web interface: Automatically enabled.

2.2.7 Keyword: scatlib

- **scatlib** *path*

  The argument *path* specifies the path to the single particle optical data set [default: *path* = 'optical_dataset/'].

  In web interface: Automatically enabled.

2.2.8 Keyword: debug

- **debug**

  Stores some internal information about the used components (netcdf files) in a file named *tmp_components.txt*. It contains info only for the last wavelength.

  In web interface: Available in expert mode.

2.2.9 Keyword: status

- **status**

  Writes the current status of the run in file *tmp_status.txt*. Might be useful in case of longer runs. This file contains the wavelength and the component currently calculated, as well as the CPU time.

  In web interface: Available in expert mode providing the CPU time after the run is finished.

3 ASCII output format

This section describes the ASCII output of the program. If the output is printed on the screen, i.e., when output ascii_file is not given, each line is preceded by the corresponding specifier.

- For **output integrated**

  The output consists of lines with 12 numbers each:

  $$\lambda\ \alpha_{ext}\ \omega_0\ g\ r_{eff}\ n\ a\ v\ M\ AE_{ext}\ AE_{sca}\ AE_{abs}$$

  where λ is the wavelength in μm, α_{ext} the extinction coefficient in m^{-1}, ω_0 the single scattering albedo, g the asymmetry parameter, r_{eff} the effective radius with the radius definition given according to the keyword size_equ, n the number density (number of particles per atmospheric volume) in m^{-3}, a the cross section density (particle cross section per atmospheric volume) in m^{-1}, v the volume density (particle volume per atmospheric volume), M the mass concentration (particle mass per atmospheric volume) in $g\,m^{-3}$, and AE_{ext}, AE_{sca}, AE_{abs} the Ångstrom exponents for extinction, scattering, and absorption.

  Note, that even if the keyword diameter is used, r_{eff} is the effective radius and not the effective diameter D_{eff}.

- For **output phase_function**

  The output consists of lines with 3 numbers each:

  $$\lambda\ \theta\ a_1$$

  where λ is the wavelength in μm, θ the scattering angle in degrees, and a_1 the phase function.

- For **output scattering_matrix**

  The output consists of lines with 8 numbers each:

  $$\lambda\ \theta\ a_1\ a_2\ a_3\ a_4\ b_1\ b_2$$

  where λ is the wavelength in μm, θ the scattering angle in degrees, and a_1 to b_2 the elements of the scattering matrix.

- For **output volume_scattering_function**

  The output consists of lines with 3 numbers each:

  $$\lambda\ \theta\ \widetilde{a}_1$$

  where λ is the wavelength in μm, θ the scattering angle in degrees, and the volume scattering function $\widetilde{a}_1$.

- For **output lidar**

  The output consists of lines with 9 numbers each:

  $$\lambda\ \alpha_{ext}\ \beta\ S\ \delta_l\ AE_{ext}\ AE_{back}\ M/\alpha_{ext}\ \beta/M$$

where λ is the wavelength in μm, α_{ext} the extinction coefficient in m^{-1}, β the backscatter coefficient in $m^{-1}sr^{-1}$, S the lidar ratio in sr, δ_l the linear depolarization ratio, AE_{ext} the Ångstrom exponent for extinction, AE_{back} the Ångstrom exponent for backscattering, M/α_{ext} the extinction to mass conversion factor in $g\,m^{-2}$, and β/M the mass to backscatter conversion factor in $m^2\,g^{-1}\,sr^{-1}$.

- For **output coeff**

  The output consists of lines with 8 numbers each:

  $$\lambda\ l\ \alpha_1^l\ \alpha_2^l\ \alpha_3^l\ \alpha_4^l\ \beta_1^l\ \beta_2^l$$

  where λ is the wavelength in μm, l is a index of the expansion coefficients, and α_1^l to β_2^l the expansion coefficients of the scattering matrix as described by Mishchenko and Travis (1998), https://doi.org/10.1016%2FS0022-4073(98)00008-9.

4 Examples

4.1 Single mode

Example with mono-modal size distribution, wavelength-independent refractive index, and spheroids of a certain aspect ratio. Particle size and refractive index affected by hygroscopic growth.

- Input file:

```
mode 1 size log_normal 0.1 2.0 1 0.005 20
mode 1 refrac 1.52 0.01
mode 1 shape spheroid oblate 1.7
mode 1 kappa 0.5
mode 1 density 2
rH 70
size_equ cs
output num_theta 4
wavelength range 0.4 0.5 0.1
output integrated
output phase_function
```

  The prefixes 'mode 1' could be removed from this example without any effect on the calculations.

- Output on the terminal:

```
integrated    4.00000E-01  3.62219E-13  9.51703E-01  7.52593E-01  ...
phase_function    4.00000E-01  0.00000E+00  5.14989E+01
phase_function    4.00000E-01  6.00000E+01  4.73597E-01
phase_function    4.00000E-01  1.20000E+02  1.64671E-01
phase_function    4.00000E-01  1.80000E+02  2.30191E-01
integrated    5.00000E-01  3.40163E-13  9.58775E-01  7.54867E-01  ...
phase_function    5.00000E-01  0.00000E+00  3.88366E+01
phase_function    5.00000E-01  6.00000E+01  5.02035E-01
phase_function    5.00000E-01  1.20000E+02  1.48386E-01
phase_function    5.00000E-01  1.80000E+02  1.93703E-01
```

- Output in file *results.integrated* when **output ascii_file** *results* is added:

```
4.00000E-01  3.62219E-13  9.51703E-01  7.52593E-01  ...
5.00000E-01  3.40163E-13  9.58775E-01  7.54867E-01  ...
```

- Output in file *results.phase_function* when **output ascii_file** *results* is added:

```
4.00000E-01  0.00000E+00  5.14989E+01
4.00000E-01  6.00000E+01  4.73597E-01
4.00000E-01  1.20000E+02  1.64671E-01
4.00000E-01  1.80000E+02  2.30191E-01
5.00000E-01  0.00000E+00  3.88366E+01
5.00000E-01  6.00000E+01  5.02035E-01
5.00000E-01  1.20000E+02  1.48386E-01
5.00000E-01  1.80000E+02  1.93703E-01
```

4.2 Multiple modes

Example of OPAC desert mixture consisting of four modes, one with spherical particles affected by hygroscopic growth and three modes with nonspherical particles with an aspect ratio distribution.

- Input file:

```
mode 1 size log_normal 0.0212 2.24 2000000000 0.005 20
mode 1 refrac file "DATAPATH/refr_water_soluble"
mode 1 shape sphere
mode 1 kappa 0.249
mode 1 density 1.8
mode 2 size log_normal 0.07 1.95 269500000 0.005 20
mode 2 refrac file "DATAPATH/refr_mineral"
mode 2 shape spheroid distr_file "DATAPATH/ar_kandler"
mode 2 kappa 0
mode 2 density 2.6
mode 3 size log_normal 0.39 2 30500000 0.005 20
mode 3 refrac file "DATAPATH/refr_mineral"
mode 3 shape spheroid distr_file "DATAPATH/ar_kandler"
mode 3 kappa 0
mode 3 density 2.6
mode 4 size log_normal 1.9 2.15 142000 0.005 60
mode 4 refrac file "DATAPATH/refr_mineral"
mode 4 shape spheroid distr_file "DATAPATH/ar_kandler"
mode 4 kappa 0
mode 4 density 2.6
rH 70
size_equ cs
wavelength range 0.5 0.7 0.1
output num_theta 361
output integrated
output header
```

  DATAPATH needs to be adjusted to the path of the MOPSMAP data directory.

- Output on the terminal:

```
#  2. column of integrated: wavelength [micrometer]
#  3. column of integrated: extinction coefficient [m^-1]
#  4. column of integrated: single scattering albedo [1]
#  5. column of integrated: asymmetry parameter [1]
#  6. column of integrated: cross section equivalent effective ...
#  7. column of integrated: number of particles per atmospheri ...
#  8. column of integrated: particle cross section per atmosph ...
#  9. column of integrated: particle volume per atmospheric vo ...
# 10. column of integrated: particle mass per atmospheric volu ...
# 11. column of integrated: angstrom exponent of the extinctio ...
# 12. column of integrated: angstrom exponent of the scatterin ...
# 13. column of integrated: angstrom exponent of the absorptio ...
integrated   5.00000E-01  1.37522E-04  8.49265E-01  7.43833E-01...
integrated   6.00000E-01  1.34457E-04  9.02721E-01  7.20565E-01...
integrated   7.00000E-01  1.32274E-04  9.17851E-01  7.11975E-01...
```