OpTool User Guide

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1. Introduction

This tool produces complex dust particle opacities right from the command line. It is derived from Michiel Min's DHS OpacityTool and also implements Ryo Tazaki's MMF theory for highly porous aggregates.

1.1. Capabilities

- stand-alone tool, fully command line driven, no input files need to be edited
- full scattering matrix output in several formats, including for RADMC-3D
- combining materials through mixing into a complex grain with porosity
- a useful collection of built-in materials for standard applications in astronomy
- an easy way to use external refractive index data
- two computational methods: (i) **DHS** (**Distribution of Hollow Spheres**) for *irregular grains* and *low-porosity* aggregates. Standard **Mie theory** for *perfect spheres* is available as a limiting case. (ii) **MMF** (**Modified Mean Field**) theory for *high-porosity/fractal aggregates*.
- Python interface module for easy postprocessing and cross-tool use.

1.2. Terms of use

optool is distributed under the MIT license and can be used, changed and redistributed freely. The relevant references for this tool are listed below. Depending on which parts of optool you are using, please reference the corresponding papers.

- optool: https://github.com/cdominik/optool.git
- DHS model for irregular grains: Min et al. 2005, A&A, 432, 909
- MMF model for aggregates: Tazaki & Tanaka 2018, ApJ 860, 79
- DIANA standard Opacities: Woitke, Min et al. 2016, A&A 586, 103
- Third party software: Toon et al. 1981, Applied Optics 20, 3657
- References to refractive index data used in your particular application.

2. Examples

A simple grain made only of the default pyroxene, for the default grain size distribution $(a^{-3.5}$ powerlaw from 0.05 to $3000\mu\text{m}$), on the default wavelength grid $(0.05\mu\text{m}$ to 1cm).

```
optool pyr
```

Include the scattering matrix in the produced output

```
optool pyr -s
```

Reproduce the DIANA standard dust model, using a specific pyroxene (70% Mg) and carbon, in a mass ratio 0.87/0.13, and with a porosity of 25%.

```
optool pyr-mg70 0.87 c 0.13 -p 0.25
```

List the built-in materials

```
optool -c
```

Add an ice mantle (built-in data from Warren+08) that is 20% of the core mass

```
optool pyr-mg70 0.87 c 0.13 -m ice-w 0.2 -p 0.25
```

Like the previous example, but use ice refractive index data from a separate file.

```
optool pyr-mg70 0.87 c 0.13 -p 0.25 -m data/ice_hudgins.dat 0.2
```

Pure ice grains in a narrow size distribution from 1 to 3 microns, with 15 sample sizes following an $f(a) \propto a^{-2.5}$ powerlaw size distribution. Also, restrict the wavelength range to $10\text{-}100\mu\text{m}$, and turn off DHS to get perfect spheres.

```
optool ice -a 1 3 2.5 15 -l 10 100 -fmax 0
```

For silicon carbide, compute the opacity of a single grains size $(2.5\mu m)$ at $\lambda=8.9\mu m$.

```
optool -a 2.5 -1 8.9 sic
```

Represent the default dust model (DIANA, you also get this when you do not give any materials at all) in 42 grain sizes, and produce input files for RADMC-3D, one for each grain size, with full scattering matrix, chopping 3 degrees from the scattering peak.

```
optool -na 42 -d -s -radmc -chop 3
```

Use MMF to compute the opacities of dust aggregates made of pyroxene monomers. Use a monomer radius of 0.3 μ m to construct aggregates with compact-volume radii between 10 and 30 μ m, and a filling factor of 5%

```
optool pyr -a 10 30 -mmf 0.3 0.05
```

As before, but fix the fractal dimension $D_f = 1.9$ instead of setting the filling factor

```
optool pyr -a 10 30 -mmf 0.3 1.9
```

3. Compiling optool

On most systems, you can download and compile optool with these simple steps, using the freely available GNU FORTRAN compiler gfortran.

```
git clone https://github.com/cdominik/optool.git
cd optool
make multi=true
```

The executable is called optool, and you should put it on your execution path. To use the Intel fortran compiler, to use multiple cores for speed (highly recommended if your system supports it), or to be able to write FITS files¹, use one or more of the following parameters during compilation:

You can also find binaries for Mac and Linux at my homepage.

4. Command line arguments

-h Show a compact help message about command line options.

4.1. Grain composition

If no composition is specified, the default is -c pyr 0.87 -c c 0.13 -p 0.25.

-c List available built-in materials (the keys for the -c and -m options).

[-c] KEY-or-FILE [MFRAC]

Specify a material to include in the grain. KEYorFILE can be the key for a builtin material, or the path to the correct lnk file. MFRAC is the *mass* fraction (default 1.0) of the material. You can give up to 10 materials to build up the grain. Mass fractions do not have to add up to one, they will be renormalized. All materials will be mixed together using the *Bruggeman* rule, and vacuum can be added through the porosity. A -c switch before each KEY-or-FILE is optional.

-m KEY-or-FILE [MFRAC]

Like -c, but place this material into the grain mantle. Multiple mantle materials will be mixed using the Bruggeman rule, and than that mix will be added to the core using the *Maxwell-Garnett* rule. The -m is *not* optional, it must be present.

-p POROSITY [P_MANTLE]

Porosity, the *volume* fraction of vacuum, a number smaller than 1. The default is 0. A single value will apply to both core and mantle, but a second value will be specific for the mantle (and may be 0).

¹This requires the cfitsio library to be installed on your system.

4.2. Grain geometry and computational method

If no method is explicitly specified, the default is **-dhs 0.8**, i.e. DHS with $f_{\text{max}}=0.8$.

-dhs [FMAX]

Use the *Distribution of Hollow Spheres* (DHS, Min+ 2005) approach to model deviations from prefect sphericity and low-porosity aggregates. Spheres with inner holes with volume fractions between 0 and f_{max} (default 0.8) are averaged to mimic irregularities. f_{max} =0 means to use solid spheres (Mie theory), i.e. perfectly regular grains. For backward compatibility, **-fmax** can be used instead of **-dhs**.

-mie

Do a standard $\it Mie$ calculation for perfect spheres. This is short for -dhs $\it 0$.

-mmf [AO [DFRAC-OR-FILL]]

Use Modified Mean Field theory (MMF, Tazaki & Tanaka 2018) to compute opacities of highly porous or fractal aggregates. -c, -m, and -p now determine the composition of monomers. A0 is the monomer radius (default 0.1μ m). Particles will be aggregates with a compact size given by the -a switch, giving rise to $N=a^3/a_0^3$ monomers. When DFRAC-OR-FILL is greater than 1, it specifies the fractal dimension. When it is less than 1, it is interpreted as the volume filling factor of the aggregates instead. The default is 0.2, corresponding to a 20% filling factor.

4.3. Grain size distribution

-a AMIN [AMAX [APOW [NA]]]

Specify (minimum) grain radius, and optionally maximum grain radius, the size distribution powerlaw and the number of size bins. You may also use options to set individual values with **-amin**, **-amax**, **-apow**, **-na**. The defaults are 0.05 μ m, 3000 μ m, 3.5, and 10 per size decade with a fixed minimum of 5, respectively. If only a single size is specified with **-a**, then $a_{max}=a_{min}$ and $n_a=1$ are implied.

4.4. Wavelength grid

-1 LMIN [LMAX [NLAM]]

Specifiy the (minimum) wavelength, and optionally the maximum wavelength and the number of wavelengths points for the construction of the wavelength grid. The default values are 0.05 μ m, 10000 μ m, and 300, respectively. You may also use the options -lmin, -lmax, and -nlam (or -nl) to set individual values. If only one wavelength is specified with -l, then $\lambda_{\text{max}} = \lambda_{\text{min}}$ and $n_{\lambda} = 1$ are implied.

-1 FILE

Read the wavelength grid from FILE. The file may start with comment lines, and the first non-comment line needs to contain the number of wavelength values in the data block below it. In the data block, the first column is expected to hold the wavelength values, in μ m. For example, an lnk file could be used here.

4.5. Controlling the output

The standard output is the file dustkappa.dat, with the opacities and the asymmetry parameter g. The following options control and extend the output.

-o [DIR]

Put the output files in directory DIR instead of the current working directory. ./output will be used if DIR is not specified.

-s [NANG]

Include the full scattering matrix in the output. NANG can optionally specify the number of equally-spaced angular grid points to cover the range of angles between 0 and 180 degrees. The default for NANG is 180 and should normally be just fine.

-chop [NDEG]

Cut out the first NDEG (2 if unspecified) degrees of the forward scattering peak and compensate by a reduction in the scattering cross section.

-d [NSUB]

Divide the computation up into NA parts to produce a file for each grain size. Each size will actually be an average over a small range of NSUB grains around the real size, to smear out resonances. The default for NSUB is 5.

-fits

Write dustkappa.fits with the absorption cross sections and scattering matrix elements, instead of ASCII output. With the -d switch, NA files will be written.

-radmc [LABEL]

RADMC-3D uses a different angular grid and normalization for the scattering matrix, so the output has to be adapted for it. The extension of the files will be changed to .inp, and if you specify LABEL, it will be used in the file name(s).

5. Material properties

optool needs refractive index data to work. For your convenience, a useful list of materials is compiled into optool. You can also find and use other data. No matter where the data is from, you should *always* cite the original laboratory papers.

5.1. Built-in materials

To access one of the built-in materials, specify the corresponding key string like pyr-mg70 instead of the path to an lnk file. In each material class I have selected a useful default, accessible with an even simpler generic key.

-c Key	-c Key	Material	State	ρ	λ_{min}	$\lambda_{\sf max}$	Reference
generic	full key			g/cm ³	μ m	μ m	
	pyr-mg100	$MgSiO_3$	amorph	2.71	0.2	500	Dorschner+95
	pyr-mg95	$Mg_{0.95}Fe_{0.05}SiO_3$	amorph	2.74	0.2	500	Dorschner+95
	pyr-mg80	$Mg_{0.8}Fe_{0.2}SiO_3$	amorph	2.9	0.2	500	Dorschner+95
pyr	pyr-mg70	$Mg_{0.7}Fe_{0.3}SiO_3$	amorph	3.01	0.2	500	Dorschner+95
	pyr-mg60	$Mg_{0.6}Fe_{0.4}SiO_3$	amorph	3.1	0.2	500	Dorschner+95
	pyr-mg50	$Mg_{0.5}Fe_{0.5}SiO_3$	amorph	3.2	0.2	500	Dorschner+95
	pyr-mg40	$Mg_{0.4}Fe_{0.6}SiO_3$	amorph	3.3	0.2	500	Dorschner+95
ens	pyr-c-mg96	$Mg_{0.96}Fe_{0.04}SiO3$	cryst	2.8	2.0	99	Jäger+98
ol	ol-mg50	MgFeSiO ₄	amorph	3.71	0.2	500	Dorschner+95
	ol-mg40	Mg _{0.8} Fe _{1.2} SiO ₄	amorph	3.71	0.2	500	Dorschner+95
for	ol-c-mg100	Mg ₂ SiO ₄	cryst	3.33	3.0	250	Steyer+74
	astrosil	MgFeSiO4	mixed	3.3	6e-5	1e5	Draine+03
С	C-Z	С	amorph?	1.8	0.05	1e4	Zubko+96
	c-p	C	amorph	1.8	0.11	800	Preibisch+93
gra	c-gra	C graphite	cryst	2.16?	0.001	1000	Draine+03
org	c-org	CHON organics	amorph	1.4	0.1	1e5	Henning+96
	c-nano	C nano-diamond	cryst	2.3	0.02	110	Mutschke+04
ice	ice-w	Water ice	cryst	0.92	0.04	2e6	Warren+08
iron	fe-c	Fe	metal	7.87	0.1	1e5	Henning+96
	fes	FeS	metal	4.83	0.1	1e5	Henning+96
	sic	SiC	cryst	3.22	0.001	1000	Laor93
cor	cor-c	Al_2O_3	cryst	4.0	0.5	40	Koike+95

5.2. External refractory index files (lnk files)

optool can use external refractive index data in files with the following format:

- The file may start with several comment lines (lines starting with !, #, or *).
- The next line contains two numbers, the number of wavelengths n_{λ} and the specific weight ρ of the material in g/cm³
- Then follow three columns of data: $\lambda[\mu m]$, and the real and imaginary parts of the refractive index, n and k.

You can find refractive index data in the Jena database, and associated with original papers in the literature. Don't forget to add the line with n_{λ} and ρ ! If for some reason it is not convenient to add that line to the file, optool will count the lines and you can specify the density after the mass fraction, like this: optool -c path/to/file.lnk 0.7 3.42. The appendix contains information on how to compile frequently-used external materials into the program.

Output files

dustkappa.dat

This is an ASCII file containing the basic opacity results. It starts with a comment section describing the dust model, followed by the format number (3, currently),

followed by the number of wavelengths in the grid, both on lines by themselves. Then follows a block with these columns:

- 1. wavelength λ [micron]
- 2. mass absorption cross section $\kappa_{\rm abs} \, [{\rm cm}^2/{\rm g}]$
- 3. mass scattering cross section $\kappa_{\rm sca}$ [cm²/g]
- 4. asymmetry parameter g

dustkapscatmat.dat

ASCII file with cross sections and full scattering matrix. The comment section at the start of the file explains the structure. See the appendix for information about the normalization of the scattering matrix. And see the <code>-radmc</code> switch which will modify the output to make sure it can be used as an input file for RADMC-3D.

dustkappa.fits

The FITS-file (ending in '.fits') is written instead of the ASCII output when using the -fits switch. It has two HDU blocks. The first block contains the cross sections per unit mass. This is an $n_{\lambda} \times 4$ matrix with these columns:

- 1. wavelengths in $[\mu m]$
- 2. mass extinction cross section $\kappa_{\rm ext}$ in [cm²/g]
- 3. mass absorption cross section $\kappa_{\rm abs}$ in [cm²/g]
- 4. mass scattering cross section $\kappa_{\rm sca}$ in [cm²/g]

The second HDU block contains the scattering matrix elements. It is a $n_{\lambda} \times 6 \times n_{\rm ang}$ matrix, containing the 6 elements of the scattering matrix for $n_{\rm ang}$ equidistant scattering angles from forward scattering (element 0) to backward scattering (element $n_{\rm ang}$ -1), for each wavelength value. The stored matrix elements are F_{11} , F_{12} , F_{22} , F_{33} , F_{34} , and F_{44} .

7. Python interface

optool comes with a python module optool.py that runs optool in the background² and puts all computed quantities as numpy arrays into a python object. This makes it straight forward to inspect and further process the output, for example to produce custom opacity files for use in an radiative transfer tool. Here is how to use the module:

```
>>> import optool
>>> p = optool.particle('~/bin/optool pyr 0.8 -m ice 0.2 -na 24 -d')
```

The argument to optool.particle() must be a valid shell command³ to run optool, if necessary with the full path to the optool binary. Depending on the presence of the

²The module runs the command as a subprocess, with output to a temporary subdirectory in the current working directory. It then reads the output files and cleans up the temporary directory unless is called with the keep keyword argument: optool.particle('optool',keep=True).

³The command may be given as string than can be split on whitespace, or, for example if the path to the binary contains whitespace, in list form ['/path/to my/command','arg1','arg2',...].

optool's -d switch, the command will produce opacities either for $n_p = 1$ particle, or for $n_p = n_a$ particles. Most of the attributes (with the exception of the global wavelength and angular grids) will therefore be arrays with the first dimension equal to n_p , even if $n_p = 1$. The object returned will have the following attributes:

Attribute	$\mathbf{Type}/\mathbf{Shape}$	Quantity		
cmd	string	The full command given in the particle() call		
radmc	boolean	Output follows RADMC conventions		
scat	boolean	Scattering matrix is available		
nlam	int	Number of wavelength points		
lam	float[nlam]	The wavelength grid		
nang	int	Number of scattering angles		
scatang	float[nang]	The angular grid		
materials	[[]]	Lists with location, m_{frac} , ρ , $material$		
np	int	Number of particles, either 1 or (with -d) n _a		
fmax	float[np]	Maximum volume fraction of vacuum for DHS		
pcore, pmantle	float[np]	Porosity of the core/mantle material		
amin, amax	float[np]	min/max grain size used for each particle		
nsub	int[np]	Number of sizes averaged for each particle.		
apow	float[np]	Negative size distribution power law (e.g. 3.5)		
a1, a2, a3	fload[np]	Mean $\langle a \rangle$, $\langle a^2 \rangle$, and $\langle a^3 \rangle$ of the particle		
kabs,ksca,kext	float[np,nlam]	Absorption, scattering/extinction cross section		
gsca	float[np,nlam]	Asymmetry parameter		
f11,, f44	<pre>float[np,nlam,nang]</pre>	Scattering matrix element F_{11}, \ldots, F_{44}		
chop	float[np]	Degrees chopped off forward scattering		
plot()	method	Plot the cross sections and matrix elements		

The optool.plot() method will produce the following plots:

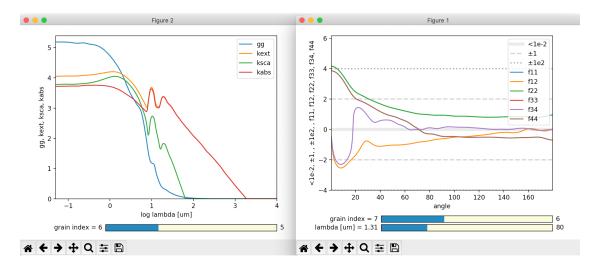


Figure 1: Screenshot of the plots created by running p.plot() on an optool particle.

- a plot showing the opacities κ_{abs} , κ_{sca} , and κ_{ext} as a function of wavelength, along with the asymmetry parameter g (on a linear y-scale). Note that the blue g curve does not have its own axis, imagine the full y axis going from 0 to 1 for g.
- a plot showing the scattering matrix elements as a function of scattering angle, with sliders to go through grain sizes and wavelengths. When interpreting the y axis, note that we plot the positive/negative \log_{10} of positive/negative matrix elements, compressing the range from 10^{-2} to 10^2 into a line (use the grey lines as a guide, ignore the y-axis labels).

8. Acknowledgments

- Charléne Lefévre for SIGMA, which triggered me to add a grain mantle using the Maxwell Garnett rule.
- Kees Dullemond for his python plotting routine viewarr (available on github).
- Jeroen Bouwman for some pointers to refractive index data.

A. Units

Due to conventions in our field, the input and output of optool uses the following units

- microns for grain sizes and wavelengths
- g/cm³ for mass densities of materials
- cm² g⁻¹ for opacities κ_{abs}, κ_{sca}, and κ_{ext}
 sr⁻¹ or cm² g⁻¹ sr⁻¹ for the scattering matrix elements, see below.

B. Scattering Matrix: The fine print

B.1. Phase function normalization

A number of different normalizations for the scattering matrix are being used in the literature and in computational tools. The differences are significant, and it is important to be aware of the choice. For optool we are using a convention (Hovenier (2004)) in which the average over all directions of the 1-1 element of the scattering matrix equals unity, i.e.

$$\oint_{(4\pi)} F_{11}(\lambda, \Theta) d\Omega = 4\pi \quad . \tag{1}$$

optool can also produce output for RADMC-3D which uses instead

$$\oint_{(4\pi)} Z_{11}(\lambda, \Theta) d\Omega = \kappa_{\rm sca}(\lambda) \quad . \tag{2}$$

The books by Bohren & Huffman and by Mishchenko use different normalizations again. As described in RADMC-3D's manual, these conventions can be matched by scaling all matrix elements with simple factors involving dust mass and wavenumber $k = 2\pi/\lambda$.

B.2. Forward-scattering peak

Particles that are much larger than the wavelength of the considered radiation can show extreme forward scattering, were much of the *scattered* radiation is sent into just a few degrees around the forward direction. This can be difficult to handle for radiative transfer codes which have limited angular resolution or limited sampling. MCMax3D has the nspike keyword to deal with this issue. Other tools (e.g. RADMC-3D) require this to be taken care of by the process that creates the opacity files. The -chop switch specifies a number of degrees around the forward scattering direction. Inside that cone, the scattering matrix gets limited to the value at the edge of the cone. To compensate and ensure energy conservation, the scattering cross section will be reduced accordingly. As a result, the radiation that would be *scattered* into this narrow range of angles will be treated as if it did have *no interaction at all* with the grain.

B.3. Angular grid

optool uses an angular grid in one degree steps from 0 to 180 degrees. The full degrees are the cell *interfaces* of that grid. optool computes the scattering matrix at the cell *midpoints*, i.e. at 0.5°, 1.5° etc to 179.5°, for a total of 180 values. The scattering matrix is normalized in this way, so that a numerical integral gives the correct result.

RADMC-3D requires the values of the scattering matrix on the cell boundaries, so at 0°, 1° etc to 180°, for a total of 181 values. For the input files for RADMC-3D, we interpolate and extend the computed values to the cell boundaries.

C. How to ingest refractive index data for another material

Using external refractive index data means that you have to keep track of where those files are. It can be convenient to compile your favorite materials into optool, so that accessing them will be as simple as using the built-in materials. Here is how to do that:

- Give your lnk file a name exactly like pyr-mg70-Dorschner1995.lnk, where the start of the name (pyr-mg70) is the key to access the material and Dorschner1995 (the text after the final -) is the reference.
- 2. Put this file into the lnk_data directory.
- 3. Optionally edit lnk_data/lnk-help.txt, so that optool -c will list the new material. Note that, in order to define generic keys, optool looks for pairs that look like genkey -> fullkey in this file.
- 4. Run make ingest to update optool_refind.f90, now including your new material
- 5. Recompile and install the code.

D. Internals

This appendix describes some key aspects of the internal workings of the code.

Refractive Index Data

Measured refractive index data is obtained from data compiled into the code, or read-in from a file. That data is then interpolated and extrapolated onto the wavelengths grid requested for the computation. Extrapolation toward short wavelengths is done keeping the refractive indices constant. Extrapolation toward long wavelength assumes that the last two measured data points define a powerlaw. Interpolation in the measured grid is done using double-logarithmic interpolation.

Mixing

Once the refractive index for all involved materials is available, the core and the mantle mixtures are created independently, using the Bruggeman rule. Mass fractions are converted into volume fractions, and porosity is implemented using vacuum as an additional material. The subroutine doing the mixing uses an iterative procedure that is very stable, also for a large number of components.

If there is a mantle, the Maxwell Garnett rule is applied with the core being treated an inclusion inside a mantle matrix.

DHS

In order to simulate irregularities in grains (irregular shapes, or the properties of low-porosity aggregates), optool averages the opacities of grains with an inner empty region, over a range of volume fractions of this inner region between 0 and $f_{\rm max}$. The subroutine used to compute the opacities and scattering matrix elements for these structures is DMiLay (Toon & Ackerman 1981). However, when the size parameter $x=2\pi a/\lambda$ exceeds a value of 10^4 , then no DHS averaging is used. A standard Mie calculation is performed , using the routine MeerhoffMie (reference missing), for a fixed size parameter of 5000, with proper scaling to the actual size of the particle.

MMF

To construct fluffy/fractal aggregates, optool needs the number of monomers N, the fractal dimension D_f , and a scaling factor k_f which are related to the radius of gyration R_g of the aggregate by

$$N = k_f \left(\frac{R_g}{a_0}\right)^{D_f} \tag{3}$$

The size a of the particles as specified by the -a switch is interpreted as the compact size of all material in the aggregate, so that simply $N=a^3/a_0^3$, where a_0 is the radius of the monomer. The average volume filling factor f can be expressed by $f=N\cdot\left(\sqrt{3/5}\,a_0/R_g\right)^3$. To determine the structure of the aggregates, the user can specify a structure parameter. If that parameter is larger than 1, it is interpreted as the fractal dimension D_f of the aggregates. Using a fixed fractal dimension means that the volume filling factor will decrease with aggregate size. As an alternative, the structure parameter can be less than 1. In that case, it is interpreted as a fixed volume filling factor f that applies to all aggregate sizes - with the implication that then the fractal dimension increases as a function of size. The fractal prefactor k_f is chosen automatically so that the asymptotic density of small aggregates is the

monomer material density. To force another value for the prefactor, it can be given explicitly as the third value of the <code>-mmf</code> option. The following table summarises the relevant equations.

	-mmf AO DF	-mmf AO FILL	-mmf AO DF KF
J	$N^{(D_f-3)/3}$	given by user	$\sqrt{27/125} k_f^{3/D_f} N^{3-1/D_f}$
D_f	given by user	$3 \ln N / \ln(N/f)$ $(5/3)^{D_f/2}$	given by user
k_f	$(5/3)^{D_f/2}$	$(5/3)^{D_f/2}$	given by user

With the structure defined, optool then applies the formalism from Tazaki & Tanaka (2018) to compute cross sections and the scattering matrix. It also computes the phase shift $\Delta \phi$ caused by the aggregate to check the validity of the scattering matrix and the asymmetry parameter. If the condition $\Delta \phi < 1$ for accurate scattering matrix results is violated, a warning will be issued. However, even then, the opacities will be applicable.

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