User Manual for DUSTY (V4)

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Abstract

DUSTY solves the problem of radiation transport in a dusty environment. The code can handle both spherical and planar geometries. The user specifies the properties of the radiation source and dusty region, and the code calculates the dust temperature distribution and the radiation field in it. The solution method is based on a self-consistent equation for the radiative energy density, including dust scattering, absorption and emission, and does not introduce any approximations. The solution is exact to within the specified numerical accuracy.

DUSTY has built in optical properties for the most common types of astronomical dust and comes with a library for many other grains. It supports various analytical forms for the density distribution, and can perform a full dynamical calculation for radiatively driven winds around AGB stars. The spectral energy distribution of the source can be specified analytically as either Planckian or broken power-law. In addition, arbitrary dust optical properties, density distributions and external radiation can be entered in user supplied files. Furthermore, the wavelength grid can be modified to accommodate spectral features. A single DUSTY run can process an unlimited number of models, with each input set producing a run of optical depths, as specified. The user controls the detail level of the output, which can include both spectral and imaging properties as well as other quantities of interest.

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1 Introduction

The code DUSTY was developed at the University of Kentucky by Željko Ivezić, Maia Nenkova, Frank Heymann, Mridupawan Deka and Moshe Elitzur for a commonly encountered astrophysical problem: radiation from some source (star, galactic nucleus, etc.) viewed after processing by a dusty region. The original radiation is scattered, absorbed and reemitted by the dust, and the emerging processed spectrum often provides the only available information about the embedded object. DUSTY can handle both planar and centrally-heated spherical density distributions. The solution is obtained through an integral equation for the spectral energy density, introduced in [10], and the spatial temperature profile is found from radiative equilibrium at every point in the dusty region. The number of independent input model parameters is minimized by fully implementing the scaling properties of the radiative transfer problem. All dimensional quantities in DUSTY are in SI units with minor exceptions: λ in μm, radius of the inner shell boundary r_1 in cm, and the luminosity of the source in $L_\odot$.

The purpose of this manual is to help users get quickly acquainted with the code. Following a short description of the installation procedure in Section 2, the input is described in full in §4, the output in Sections 5 and 6 for, respectively, spheres and slabs. Finally, Section 7 describes the user control of DUSTY

1.1 Major Changes

This new version of DUSTY (`dusty.f90`, internally known as V4) is faster than its previous public release (internally known as version V2), particularly for the slab case. Because of the addition of some new features, the structure of the input has changed and old input files will not run on the current version. The major changes are:

- **External radiation for spherical case:** The heating radiation can now come from external, isotropic radiation rather than a central source. The previous version had only the central source option.

- **Input files format** has been changed. Descriptive keywords are now used wherever possible instead of numerical flags. For example, the slab geometry is now specified with `Geometry = SLAB` instead of the previously used numerical flag `density type = 0`. Details of the format of input files and the available options are described in Section 4.

  Note: The keywords can be entered in either upper or lower case, and each keyword must be followed by a blank space.

- **Sublimation temperature as dust property:** The input file has to include the dust sublimation temperature as one of the dust properties. Details of the dust properties and the available options are described in Section 4.3.2.

- **Master Input File:** The name of the master input file has changed from `dusty.inp` to `dusty.mas`. Names of the input files listed in a master file must now include explicitly the extension `.inp`; this extension was omitted in the previous versions of the master file.

- **Optional Arguments:** DUSTY can now be launched with an optional argument that allows an arbitrary location for the master input as well as simultaneous launching of multiple occurrences of DUSTY; see §3 for details.

2 Installation

Download the file `dusty.tar`[1] and then untar it, maintaining the directory structure. The gzipped file contains the following:

- The source code `dusty.f90`

- The file `userpar.inc` with user adjustable array sizes

- The subdirectory `data` with various data files such as the wavelength grid `lambda_grid.dat`, optical properties of different dust models, etc.

- The master input file `dusty.mas`.

- Sample input files in the subdirectories of `examples`. They are listed in the master input file, `dusty.mas`, together with brief descriptions and can be used as templates.

  All input files contain explanations and examples of the various options. Their corresponding outputs are produced in the same subdirectory `examples` and can be compared with the files in each corresponding `output` subdirectory.

[1] https://github.com/ivezic/dusty/tree/master/release/dusty.tar

DUSTY is written in standard FORTRAN 90. It was developed under gnu-fortran and can be compiled with, for example,

```
gfortran -O3 -lgomp -fopenmp -o dusty.exe dusty.f90
```

The options listed here ensure high-optimization (`-O3`) and parallel computation (`-lgomp -fopenmp`) on multi-core machines. This operation can be performed instead with the supplied `Makefile` on Unix machines or `compile.bat` on Windows machines. If the compilation is successful you can immediately proceed to run the executable `dusty.exe` without any further action. It should produce the output files `sphere#.out` and `slab#.out`, printed in appendices C and D, respectively.

2.1 Numerical Test

Due to the complications inherent to the numerical solution of radiative transfer, it is a good idea to perform a numerical test of DUSTY for a case with a known exact solution. Any dust distribution, irrespective of geometry and optical depth, embedded in an external black-body radiation field with a given temperature should equilibrate with that temperature when there is no scattering (only absorption). This numerical test can be performed with the two included input files `sphere_bb.inp` and `slab_bb.inp`, for sphere and slab respectively; just uncomment these input files in the supplied `dusty.mas`.

3 Launching DUSTY

DUSTY must be launched from the default directory that contains the executable, or a link to it. A single DUSTY run can process an arbitrary number of models. To accomplish this, DUSTY's default input is the master input file `dusty.mas` that lists the actual input files for all models. When DUSTY is invoked without parameters, `dusty.mas` must be kept in the DUSTY default directory. The very first line of the master input contains the statement `verbose = v`, where `v` sets the level of DUSTY's verbosity during execution. With `verbose = 1` DUSTY will output to the screen a minimal progress report of its execution. With `verbose = 2` you get a more detailed report that allows tracing in case of execution problems. `verbose = 0` suppresses all messages. The messages are printed to the standard output device with the FORTRAN statement `write(*)`. If you suspect that your system may not handle this properly, choose `verbose = 0`.

Following the verbosity statement, the master input file lists the actual input files for the run. Each input filename must be listed on a separate line and have the form `fname.inp`, where `fname` is arbitrary and can include the full path.[2] A single run can thus produce output models in different directories. Since FORTRAN requires termination of input records with a carriage return, make sure you press the "Enter" key after every filename you enter, especially if it is in the last line of `dusty.mas`. Empty lines are ignored, as is all text following the '`%`' sign (as in TEX). This enables you to enter comments and conveniently switch on and off the running of any particular model.

The sample `dusty.mas`, supplied with the program, points to a number of actual input files. Of those, only `sphere1.inp` and `slab1.inp` will be executed, since the others are commented out, providing samples of DUSTY's simplest possible input and output. Once they have been successfully

[2] In previous versions of DUSTY, the extension `.inp` was omitted from the listing in the master input file.

run you may wish to remove the '%' signs from the other entries, which demonstrate more elaborate input and output, and check the running of a full sequence. Your output can be verified against the corresponding sample output files accessible on DUSTY's homepage. Of special importance are the sample input files `sphereBB.inp` and `slabBB.inp`, which place a sphere and a slab in a black-body radiation bath and turn off the dust scattering (by using the data file `ism-noscatt.dat`). In both cases, the dust temperature must equilibrate with that of the background bath, providing a numerical check of your system.

3.1 Optional Arguments

DUSTY can be launched with an optional argument, which can be either `fname.mas` or `fname.inp`, where `fname` is an arbitrary file name that can also contain a full path. When the file extension is `.mas`, DUSTY uses this as its master input file for the run; i.e., neither name nor location of the master input are constrained in this case. This allows simultaneous launching of multiple occurrences of DUSTY, each with a different master input file. When the file extension of the optional argument is `.inp`, DUSTY will run a single input file without any master file. This can be useful for a quick check of an input file or for running simultaneously multiple instances of DUSTY. When using the `.inp` option, the default verbosity level is 2. A lower level can be obtained by entering it as an optional second argument; for example, the command

```
dusty fname.inp 0
```

will trigger a `verbose = 0` DUSTY run with the input file `fname.inp`. **Note: When** DUSTY **is invoked without an argument it expects the default master input file** `dusty.mas` **in the default directory**.

4 Input

Each model is characterized by properties of the radiation source and the dusty region, and DUSTY produces a set of up to 999 solutions for all the optical depths specified in the input. The output file for `fname.inp` is `fname.out`, containing a summary of the run and a table of the main output results. Additional output files containing more detailed tables of radiative and radial properties may be optionally produced.

The input file has a free format, text and empty lines can be entered arbitrarily. All lines that start with the '*' sign are copied to the output, and can be used to print out notes and comments. This option can also be useful when the program fails for some mysterious reason and you want to compare its output with an exact copy of the input line as it was read in before processing by DUSTY. The occurrence of relevant numerical input, which is entered in standard FORTRAN conventions, is flagged by the equal sign '='. The only restrictions are that all required input entries must be specified, and in the correct order; the most likely source of an input error is failure to comply with these requirements. Recall, also, that FORTRAN requires a carriage return termination of the file's last line if it contains relevant input. Single entries are always preceded by the equal sign, '=', and must be padded by blanks on both sides; the terminating blank can be optionally preceded with a comma. For example: `T = 10,000 K` as well as `Temperature = 1.E4 degrees` and simply `= 10000.00` are all equivalent, legal input entries (note that comma

separations of long numbers are permitted). Some input is entered as a list, in which case the first member is preceded by '=' and each subsequent member must be preceded by a blank (an optional comma can be entered before the blank for additional separation); for example, `Temperatures = 1E4, 2E4 30,000`. Because of the special role of '=' as a flag for input entry, care must be taken not to introduce any '=' except when required. All text following the `'%'` sign is ignored (as in TEX) and this can be used to comment out material that includes '=' signs. For example, different options for the same physical property may require a different number of input entries. By commenting out with `'%'`, all options may be retained in the input file with only the relevant one switched on.

The input contains three types of data — physical parameters, numerical accuracy parameters, and flags for optional output files. The physical parameters include characteristics of the external radiation, properties of the dust grains, and the envelope density distribution. Detailed description of the program input follows, including examples marked with the '•' sign. Each example contains a brief explanation, followed by sample text typeset in `typewriter font` as it would appear in the input file. The sample input files supplied in directory `examples` are heavily commented to ease initial use and can be used as templates.

4.1 Geometry

DUSTY can handle two types of geometry — spherical and planar (slab). Each DUSTY run involves one type of geometry, and this is the first input parameter. The input

```
GEOMETRY = SLAB
```

invokes the slab geometry. Because of the planar symmetry, the density profile is irrelevant in this case: location in the slab is uniquely specified by the optical depth from the surface; the actual density distribution is irrelevant to the radiative transfer problem. Unlike the spherical case, there is no reference to spatial variables since the problem can be solved fully in optical-depth space. Thus the slab requires no additional input regarding the geometry.

The spherical geometry is invoked by the input statement

```
GEOMETRY = SPHERE
```

Beginning with this version, DUSTY provides a choice between two different numerical methods for solution of the spherical problem. The above input invokes an accelerated Λ-iteration scheme, which is now DUSTY's standard method. Optionally, the spherical geometry can instead be invoked with

```
GEOMETRY = SPHERE_MATRIX
```

which triggers the matrix inversion direct-method [21] that was used in all previous versions of DUSTY. This method is applicable only when the external radiation comes from a central point source (see §4.2 below). In that case it can be more efficient at high optical depths (> 100) and may be tried when the other method encounters numerical difficulties.

Because of the curvature, the dust radial density distribution is required and must be specified in the following input. The dust density distribution is specified in terms of the scaled radius

$$y = \frac{r}{r_1}$$

where r_1 is the shell inner radius. This quantity is irrelevant to the radiative transfer problem [10], therefore it is not entered (r_1 scales with the luminosity L as $L^{1/2}$ when all other parameters are held fixed. The explicit relation is provided as part of DUSTY's output; see §5.1.) The density distribution is described by the dimensionless profile $\eta(y)$, which DUSTY normalizes according to $\int \eta dy = 1$. Note that the shell inner boundary is always $y = 1$. Its outer boundary in terms of scaled radii is the shell relative thickness, and is specified as part of the definition of η.

DUSTY provides three methods for entering the spherical density distribution: prescribed analytical forms, hydrodynamic calculation of winds driven by radiation pressure on dust particles, and numerical tabulation in a file.

4.1.1 Analytical Profiles

DUSTY can handle three types of analytical profiles: piecewise power-law, exponential, and an analytic approximation for radiatively driven winds. The last option is described in the next subsection on winds.

- Piecewise power law:

$$\eta(y) \propto \begin{cases} y^{-p(1)} & 1 \le y < y(1) \\ y^{-p(2)} & y(1) \le y < y(2) \\ y^{-p(3)} & y(2) \le y < y(3) \\ & \vdots \\ y^{-p(N)} & y(N-1) \le y \le y(N) \end{cases}$$

  After the option selection, the number N is entered, followed by a list of the break points $y(i)$, $i = 1 \ldots N$, and a list of the power indices $p(i)$, $i = 1 \ldots N$. The list must be ascending in y. Examples:

  - Density falling off as y^{-2} in the entire shell, as in a steady-state wind with constant velocity. The shell extends to 1000 times its inner radius:

```
density type = POWD ;     N = 1;    Y = 1.e3;     p = 2
```

  - Three consecutive shells with density fall-off softening from y^{-2} to a constant distribution as the radius increases by factor 10:

```
     density type = POWD
                N = 3
transition radii = 10   100    1000
power indices    = 2     1       0
```

- Exponentially decreasing density distribution

$$\eta \propto \exp\left(-\sigma \frac{y-1}{Y-1}\right) \tag{1}$$

where Y is the shell's outer boundary and σ determines the fall-off rate. Following the option flag, the user enters Y and σ. Example:

  - Exponential fall-off of the density to e^{-4} of its inner value at the shell's outer boundary $Y = 100$:

```
density type = EXPD ; Y = 100; sigma = 4
```

4.1.2 Radiatively Driven Winds

Two more density distribution options are offered for the modeling of objects such as AGB stars, where the envelope expansion is driven by radiation pressure on the dust grains. DUSTY can compute the wind structure by solving the hydrodynamics equations, including dust drift and the star's gravitational attraction, as a set coupled to radiative transfer. This numerical solution is triggered with `density type = RDW`, while `density type = RDW_Analytic` utilizes an analytic approximation for the dust density profile which is appropriate in most cases and offers the advantage of a much shorter run time.

- An exact calculation of the density structure from a full dynamics calculations (see [7, 3] and references therein). The calculation is performed for a typical wind in which the final expansion velocity exceeds 5 km s^{-1}, but is otherwise arbitrary. The only input parameter that needs to be specified is the shell thickness $Y = r_{\rm out}/r_1$.

  - Numerical solution for radiatively driven winds, extending to a distance 10^4 times the inner radius:

```
density type = RDW ;      Y = 1.e4
```

  The steepness of the density profile near the wind origin increases with optical depth, and with it the numerical difficulties. DUSTY handles the full dynamics calculation for models that have $\tau_V \lesssim 1{,}000$, corresponding to $\dot{M} \sim 4{\times}10^{-4}\ M_\odot$ yr^{-1}.

- When the variation of flux-averaged opacity with radial distance is negligible, the problem can be solved analytically [3]. In the limit of negligible drift, the analytic solution takes the form

$$\eta \propto \frac{1}{y^2}\left[\frac{y}{y-1+(v_1/v_e)^2}\right]^{1/2} \tag{2}$$

  This density profile provides an excellent approximation under all circumstances to the actual results of detailed numerical calculations (previous option). The ratio of initial to final velocity, $\epsilon_v = v_1/v_e$, is practically irrelevant as long as $\epsilon_v \lesssim 0.2$. The selection `density type = RDW_Analytic` invokes this analytical solution with the default value $\epsilon_v = 0.2$. As for the previous option, the only input parameter that needs to be specified in this case is the outer boundary Y.

– Analytical approximation for radiatively driven winds, the shell relative thickness is $Y = 10^4$:

```
density type = RDW_Analytic ;      Y = 1.e4
```

Run times for this option are typically 2–3 times shorter and it can handle larger optical depths than the previous one. Although this option suffices for the majority of cases of interest, for detailed final fitting you may wish to switch to the former.

4.1.3 Tabulated Profiles

Arbitrary density profiles can be entered in tabulated form in a file. The tabulation could be imported from another dynamical calculation (e.g., star formation), and DUSTY would produce the corresponding IR spectrum. The file `collapse.dat` is supplied with DUSTY and contains tabulation of the profile $\eta \propto y^{-3/2}$, corresponding to steady-state accretion to a central mass. It can be invoked as follows:

```
density type     = USR_SUPPLD
profile filename = data/collapse.dat
```

This input file can optionally start with an arbitrary number of header lines, in which case they must be terminated by a line containing '>' in the first column. This header section is followed by a two-column tabulation of radius and density, ordered in increasing radius. In the case of a central heating source whose flux scale is specified through the dust temperature T_1 on the inner boundary (see §4.2.2 below), the inner radius (first entry) must correspond to that temperature. Otherwise, the units of both radius and density are arbitrary; DUSTY will transform both to dimensionless variables. The number of entry data points is limited to a maximum of 1,000 but is otherwise arbitrary. DUSTY will transform the table to its own radial grid, with typically $\sim$ 20–30 points. Note that DUSTY may have trouble handling density profiles that have large derivatives, or that drop to 0 at some radii. The cubic spline method employed by DUSTY significantly reduces the number of radial grid points, but is not capable of describing sharp features.

In all cases, care must be taken that η not become so small that roundoff errors cause spline oscillations and decrease accuracy. To avoid such problems, DUSTY will stop execution with a warning message whenever η dips below 10^{-15} or its dynamic range exceeds 10^{15}. This is particularly pertinent for very steep density profiles, where the outer boundary should be chosen with care.

4.2 External Radiation

DUSTY can handle various combinations of heating sources. In the spherical case, the external radiation can come from either a point source at the center of the dust distribution or isotropic radiation from outside the shell. In the slab case, radiation always enters from the left side, with optional illumination also from the right side. All combinations are triggered with `ON/OFF` flags in the input file. When a radiation field is turned `ON`, this flag must be followed by specifications of its spectral shape and strength. These options are described separately in the following subsections.

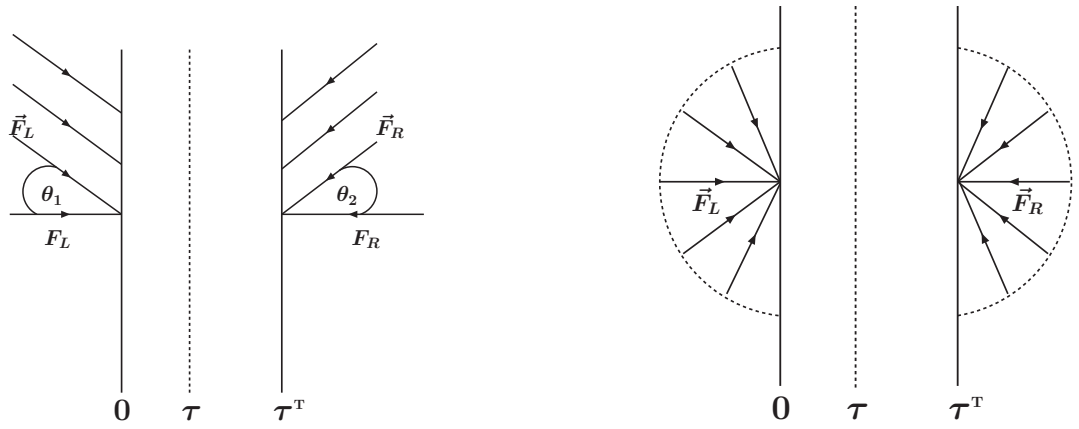

Figure 1: External heating of a slab. *Left*: Directional illumination from both sides. *Right*: Isotropic radiation on both sides. Note that the total flux vanishes in both cases whenever $\vec{F}_{\mathrm{L}} = \vec{F}_{\mathrm{R}}$.

- In the spherical case, the first flag is for a central source. For example,

  ```
  central = ON
  ```

  is to be followed by input for spectral shape and strength of the central source. Afterwards comes the flag for the external radiation; for example

  ```
  external = OFF
  ```

  ends the external radiation input in this case. **NOTE: Only one source of radiation, either internal or external, is allowed in the spherical case**

- In the slab case, both isotropic radiation and parallel-ray illumination maintain the planar symmetry (see figure 1). Therefore, the radiation angular distribution must be specified first, before its spectral shape and strength. Since the left-side radiation is always present, the first input is for its angular distribution:

  ```
  angular distribution = ISOTROPIC
  ```

  for isotropic radiation or

  ```
  angular distribution = DIRECTIONAL
  illumination angle   = 60 degrees
  ```

  for the parallel-rays case; because of numerical considerations, only $\theta \leq 85^\circ$ is allowed. Each case is to be followed by input for the spectral shape and strength of the left-side source. The optional right-side illumination is specified with an `ON/OFF` flag. For example,

  ```
  right = OFF
  ```

indicates left-side illumination only, while additional radiation on the right is specified with

```
right = ON
angular distribution = DIRECTIONAL
illumination angle   = 30 degrees
```

followed by input for the spectral shape and strength of the right-side source. You can mix the types of radiation, e.g., directional on the left and isotropic on the right. Care must be taken to supply the proper illumination angle ($\leq 85°$) for each directional component.

Each external radiation component that is `ON` must be additionally specified by its spectral shape and strength. Next we describe the input specifications for these properties.

4.2.1 Spectral Shape of External Radiation

Because of scale invariance, the only property of the external radiation that must be always specified is its spectral shape (see [10]). Six different selected input options are available in DUSTY. Three involve entry in analytical form: (1) a combination of black-bodies, (2) an empirical expression devised by Engelke [4] and Marengo [16], and (3) broken power law. The other three are for entry in numerical form as a separate user-supplied input file which lists either (4) λF_λ ($= \nu F_\nu$) or (5) F_λ, or (6) F_ν vs λ. Here λ is wavelength in μm and ν the corresponding frequency, and F_λ or F_ν is the external flux density in arbitrary units. The detailed properties of the different options are as follows:

- A combination of up to 10 black bodies, each described by a Planck function of a given temperature. Following the spectral flag, the number of black bodies is specified, followed by a list of the temperatures. When more then one black-body is specified, the temperature list must be followed by a list of the fractional contributions of the different components to the overall spectral shape.

  – A single black body:

  ```
  Spectral Shape = BLACK_BODY
    Number of BB = 1
     Temperature = 10,000 K
  ```

  Note that this could also be entered on a single line as

  ```
  type = BLACK_BODY , N = 1, T = 1E4
  ```

  – Two black bodies, e.g. a binary system, with the first one contributing 80% of the total luminosity (note that the distance between the stars must be sufficiently small that the assumption of a central point source remain valid):

  ```
  Spectral Shape = BLACK_BODY
    Number of BB = 2
    Temperatures = 10,000, 2,500 K
    Luminosities = 4, 1
  ```

- Engelke-Marengo function. This expression improves upon the black-body description of cool star emission by incorporating empirical corrections for the main atmospheric effects. Engelke [4] found that changing the temperature argument of the Planck function from T to $0.738T[1+79450/(\lambda T)]^{0.182}$ adequately accounts for the spectral effect of H^-. Massimo Marengo [16] devised an additional empirical correction for molecular SiO absorption around 8 μm, and has kindly made his results available to DUSTY. The selection of this combined Engelke-Marengo function requires as input the temperature and the relative (to the continuum) SiO absorption depth in %.

  – Stellar spectrum parametrized with Engelke–Marengo function:

```
Spectral Shape = ENGELKE_MARENGO
   Temperature = 2500 K
SiO absorption depth = 10 percents
```

- Broken power law of the form

$$\lambda F_\lambda \propto \begin{cases} 0 & \lambda \le \lambda(1) \\ \lambda^{-k(1)} & \lambda(1) < \lambda \le \lambda(2) \\ \lambda^{-k(2)} & \lambda(2) < \lambda \le \lambda(3) \\ \vdots & \\ \lambda^{-k(N)} & \lambda(N) < \lambda \le \lambda(N+1) \\ 0 & \lambda(N+1) < \lambda \end{cases}$$

  In this case, after the option selection the number N is entered, followed by a list of the break points $\lambda(i)$, $i = 1 \ldots N+1$, in μm and a list of the power indices $k(i)$, $i = 1 \ldots N$. It is important to list the wavelengths $\lambda(i)$ in increasing order.

  – A flat spectrum confined to the range 0.1–1.0 μm:

```
Spectral Shape = POWER_LAW
             N = 1
        lambda = 0.1, 1 micron
             k = 0
```

    All spectral points entered outside the range covered by DUSTY's wavelength grid are ignored. If the input spectrum does not cover the entire wavelength range, all undefined points are assumed zero.

- Stellar spectrum tabulated in a file. The filename for the input spectrum must be entered separately in the line following the numerical flag. This input file can optionally start with an arbitrary number of header lines, in which case they must be terminated by a line containing '>' in the first column. This header section is followed by a two-column tabulation of λ and λF_λ, where λ is in μm and λF_λ is in arbitrary units. The number of entry data points is limited to a maximum of 10,000 but is otherwise arbitrary. The tabulation must be ordered in wavelength but the order can be either ascending or descending. If the shortest

tabulated wavelength is longer than 0.01 μm, the external flux is assumed to vanish at all shorter wavelengths. If the longest tabulated wavelength is shorter than 3.6 cm, DUSTY will extrapolate the rest of the spectrum with a Rayleigh-Jeans tail.

  - Spectral Shape tabulated in file `quasar.dat`:
    `Spectral Shape = FILE_LAMBDA_F_LAMBDA`
    `filename = data/quasar.dat`

- Stellar spectrum read from a file as in the previous option, but F_λ is specified (in arbitrary units) instead of λF_λ.

  - Kurucz model atmosphere tabulated in file `kurucz10.dat`:
    `Spectral Shape = FILE_F_LAMBDA`
    `filename = data/kurucz10.dat`

- Stellar spectrum read from a file as in the previous option, but F_ν is specified (in arbitrary units) instead of F_λ.

  - Spectral Shape tabulated in file `quasar_Fnu.dat`:
    `Spectral Shape = FILE_F_NU`
    `filename = data/quasar_Fnu.dat`

Note that in the last three entry options, the filename for the input spectrum must be entered separately in the line following the name flag. Optionally, you may separate the flag line and the filename line by an arbitrary number of lines that are either empty or commented out (starting with '`%`'). The files quasar.dat, kurucz10.dat and quasar_Fnu.dat are distributed with DUSTY.

4.2.2 Input Radiation Strength

There are five different ways to enter the scale of the input radiation: (1) bolometric flux, (2) luminosity and distance, (3) energy density, (4) dilution factor for black body radiation, and (5) dust temperature on the illuminated boundary. Option (5) is applicable only in the cases of central source for the spherical geometry and left side illumination for the slab case. Examples of these options follow.

- The input radiation strength can be specified by its bolometric flux, in W/m^2, on the illuminated surface:

```
Scale:    type of entry = FLUX
                     Fe = 2.6E4 W/m^2
```

  In the spherical case this option can be used only for a central source, and `Fe` is the illuminating flux on the inner boundary. In the slab case this option applies only for directional illumination, and `Fe` is the flux entering from the left.

- Alternatively, the heating flux can be specified by entering the source luminosity (in $L_\odot$) and its distance (in cm) from the illuminated boundary:

```
Scale:     type of entry = LUM_R1
                      L = 1.0E4       % Luminosity [in Lo] and
                      d = 3.43e14 cm  % distance [cm] from the source
```

  This method is equivalent to the previous one with $F_\mathrm{e} = L/4\pi d^2$.

- The heating radiation scale can be specified instead by its energy density at the illuminated boundary:

```
Scale:     type of entry = ENERGY_DEN       % Energy density of
                     J = 2.5e-5 W/m^2       % the ext. radiation
```

  This type of entry is essential in the case of isotropic illumination (in both the spherical and planar cases), where the flux is zero and the previous two methods cannot be used.

- Since the black-body function carries an absolute scale, its flux level can be specified by a dilution factor (≤ 1):

```
Scale:   type of entry = DILUTN_FAC     % dilution factor
                       W = 1.0e-5
```

  This type of entry can be used *only* when the spectral shape is a combination of one or more black-bodies. In the case of multiple components, the dilution factor refers to the black-body that carries the highest specified luminosity.

- Thanks to scaling ([10]), the dust temperature on the illuminated boundary can be specified instead of the heating radiation strength at that position. This option can be used only when there is one external source of heating radiation—a central source in the spherical case, left-side illumination in the slab case:

```
Scale:     type of entry = T1        % Td at the illuminated boundary
                    Td = 1000  K
```

  The input `Td` is the dust temperature on the inner boundary of the spherical shell or the left surface of the slab. The corresponding external bolometric flux on the illuminated surface is computed by DUSTY and listed in the default output file. In principle, different types of grains can have different temperatures at the same location. However, DUSTY currently treats mixtures as single-type grains whose properties average the actual mix, therefore only one temperature is specified.

4.3 Dust Properties

Dust optical properties are described by the dust absorption and scattering cross-sections, which depend on the grain size and material. Currently, DUSTY supports only single-type grains, namely, a single size and chemical composition. Grain mixtures can still be treated, simulated by a single-type grain constructed from an appropriate average. This approximation will be removed in future releases which will provide full treatment of grain mixtures.

4.3.1 Chemical Composition

DUSTY contains data for the optical properties of six common grain types. In models that utilize these standard properties, the only input required is the fractional abundance of the relevant grains. In addition, optical properties for other grains can be supplied by the user. In this case, the user can either specify directly the absorption and scattering coefficients or have DUSTY calculate them from provided index of refraction. The various alternatives are selected by a flag, as follows:

- DUSTY contains data for six common grain types: 'warm' and 'cold' silicates from Ossenkopff et al ([18], `Sil-Ow` and `Sil-Oc`); silicates and graphite grains from Draine and Lee ([2], `Sil-DL` and `grf-DL`); amorphous carbon from Hanner ([5], `amC-Hn`); and SiC by Pègouriè ([19], `SiC-Pg`). Fractional number abundances must be entered for all these grain types, in the order listed.

  – Mixture containing only dust grains with built-in data for optical properties:

  ```
  optical properties index = COMMON_GRAIN_COMPOSITE
  Abundances for supported grain types, standard ISM mixture:

      Sil-Ow  Sil-Oc  Sil-DL  grf-DL  amC-Hn   SiC-Pg
  x =  0.00    0.00    0.53    0.47    0.00     0.00
  ```

  The overall abundance normalization is arbitrary. In this example, the silicate and graphite abundances could have been entered equivalently as 53 and 47, respectively.

- With this option, the user can introduce up to ten additional grain types on top of those built-in. First, the abundances of the six built-in types of grains are entered as in the previous option. Next, the number (≤ 10) of additional grain types is entered, followed by the names of the data files, listed separately one per line, that contain the relevant optical properties. These properties are specified by the index of refraction, and DUSTY calculates the absorption and scattering coefficients using Mie theory. Each data file can optionally start with an arbitrary number of header lines, in which case they must be terminated by a line containing '>' in the first column. This header section is followed by a three-column tabulation of wavelength in μm, and real (`n`) and imaginary (`k`) parts of the index of refraction. The number of table entries is arbitrary, up to a maximum of 10,000. The tabulation must be ordered in wavelength but the order can be either ascending or descending. DUSTY will linearly interpolate the data for `n` and `k` to its built-in wavelength grid. If the supplied data does not fully cover DUSTY's wavelength range, the refraction index will be assumed constant in the unspecified range, with

a value equal to the corresponding end point of the user tabulation. The file list should be followed by a list of abundances, entered in the same order as the names of the corresponding data files.

  - Draine & Lee graphite grains with three additional grain types whose `n` and `k` are provided by the user in data files `amC-zb1.nk`, `amC-zb2.nk` and `amC-zb3.nk`, distributed with DUSTY. These files tabulate the most recent properties for amorphous carbon by Zubko et al [22]:

```
Optical properties index = COMMON_AND_ADDL_GRAIN_COMPOSITE
Abundances of built-in grain types:
      Sil-Ow  Sil-Oc  Sil-DL  grf-DL amC-Hn SiC-Pg
  x =  0.00    0.00    0.00    0.22   0.00  0.00

Number of additional components = 3, properties listed in files
                  amC-zb1.nk
                  amC-zb2.nk
                  amC-zb3.nk
Abundances for these components = 0.45, 0.10, 0.23
```

- This option is similar to the previous one, only the absorption and scattering coefficients are tabulated instead of the complex index of refraction, so that the full optical properties are directly specified and there is no further calculation by DUSTY. The data filename is listed in the line following the option flag. This input file can optionally start with an arbitrary number of header lines, in which case they must be terminated by a line containing '>' in the first column. This header section is followed by a three-column tabulation of wavelength in μm, absorption ($\sigma_{\rm abs}$) and scattering ($\sigma_{\rm sca}$) cross sections. Units for $\sigma_{\rm abs}$ and $\sigma_{\rm sca}$ are arbitrary, only their spectral variation is relevant. The number of entries is arbitrary, with a maximum of 10,000. The handling of the wavelength grid is the same as in the previous option.

  - Absorption and scattering cross sections from the file `ism-stnd.dat`, supplied with DUSTY, listing the optical properties for the standard interstellar dust mixture:

```
Optical properties index = TABULATED
X-sections input file    = data/ism-stnd.dat
```

DUSTY's distribution includes a library of data files with the complex refractive indices of various compounds of common interest. This library is described in appendix E.

4.3.2 Sublimation temperature

The dust sublimation temperature specifies the highest temperature at which the dust grains can exist:

```
Sublimation Temperature = 1500K
```

If DUSTY's solution includes dust at higher temperatures, DUSTY will print a warning message on the screen and in `fname.out`. The Sections 5.1 (sphere) and 6.1 (slab) describe the file `fname.out` in detail.

4.3.3 Grain Size Distribution

The grain size distribution must be specified only when the previous option was set to `COMMON_GRAIN_COMPOSITE` or `COMMON_AND_ADDL_GRAIN_COMPOSITE`. When the dust cross sections are read from a file (previous option set at `TABULATED`), this particular option is skipped.

DUSTY recognizes two distribution functions for grain sizes $n(a)$ — the MRN [17] power-law with sharp boundaries

$$n(a) \propto a^{-q} \qquad \text{for} \quad a_{\min} \le a \le a_{\max} \tag{3}$$

and its modification by Kim, Martin and Hendry [15], which replaces the upper cutoff with a smooth exponential falloff

$$n(a) \propto a^{-q} e^{-a/a_0} \qquad \text{for} \quad a \ge a_{\min} \tag{4}$$

DUSTY contains the standard MRN parameters $q = 3.5$, $a_{\min} = 0.005$ μm and $a_{\max} = 0.25$ μm as a built-in option. In addition, the user may select different cutoffs as well as power index for both distributions.

- This is the standard MRN distribution.

  ```
  Size distribution = MRN
  ```

  No input required other than the option flag.

- Modified MRN distribution. The option flag is followed by listing of the power index q, lower limit $a_{\min}$ and upper limit $a_{\max}$ in μm.

  - Standard MRN distribution can be entered with this option as:

    ```
    Size distribution = MODIFIED_MRN
    q = 3.5, a(min) = 0.005 micron, a(max) = 0.25 micron
    ```

  - Single size grains with $a = 0.05$ μm:

    ```
    Size distribution = MODIFIED_MRN
                    q = 0 (it is irrelevant in this case)
              a(min) = 0.05 micron
              a(max) = 0.05 micron
    ```

- KMH distribution [15]. The option flag is followed by a list of the power index q, lower limit $a_{\min}$ and the characteristic size a_0 in μm.

  - Size distribution for grains in the dusty envelope around IRC+10216 as obtained by Jura [14] and verified in Ivezić & Elitzur [9]:

    ```
    Size distribution = KMH
    q = 3.5, a(min) = 0.005 micron, a0 = 0.2 micron
    ```

4.4 Optical Depth

For a given set of the parameters specified above, DUSTY will generate up to 999 models with different overall optical depths. The list of optical depths can be specified in two different ways. DUSTY can generate a grid of optical depths spaced either linearly or logarithmically between two end-points specified in the input. Alternatively, an arbitrary list can be entered in a file.

- Optical depths covering a specified range in linear steps: Following the option selection, the fiducial wavelength λ_0 (in μm) of optical depth τ_0 is entered. The τ_0 grid is then specified by its two ends and the number of points (≤ 999).

  – Models with 2.2 μm optical depths including all the integers from 1 to 100:

  ```
  tau grid = LINEAR
  lambda0  = 2.2 micron
  tau(min) = 1; tau(max) = 100
  number of models = 100
  ```

- Same as the previous option, only the τ_0 range is covered in logarithmic steps:

  – Three models with visual optical depth $\tau_V = 0.1$, 1 and 10:

  ```
  tau grid = LOGARITHMIC
  lambda0  = 0.55 micron
  tau(min) = 0.1; tau(max) = 10
  number of models = 3
  ```

- Optical depths list entered in a file: The file name is entered on a single line after the option selection. The supplied file can optionally start with an arbitrary number of header lines, in which case they must be terminated by a line containing '>' in the first column. This header section is followed by the fiducial wavelength λ_0, preceded by the equal sign, '='. The list of optical depths, one per line up to a maximum of 999 entries, is entered next in arbitrary order. DUSTY will sort and run it in increasing τ_0.

  – Optical depths from the file `taugrid.txt`, supplied with the DUSTY distribution:

  ```
  tau grid = USER_SUPPLIED  % grid supplied in file:
  data/taugrid.dat
  ```

  The file `taugrid.dat` is used in the sample input files `slab2.inp` and `sphere3.inp`.

4.5 Numerical Accuracy and Internal Bounds

DUSTY's accuracy is controlled by internal convergence criteria, as well as the density of the wavelength and spatial grids employed in the computations. The wavelength grid can be modified by users to meet their specific needs (see §7.2) and it does not change during execution. Flux conservation is controlled by the density of the spatial grids. These are automatically generated and refined until the fractional error of flux conservation at every grid point is less than $q_{\rm acc}$, entered as

```
accuracy for flux conservation = 0.1
```

This accuracy is calculated from $(F_{\max} - F_{\min})/(F_{\max} + F_{\min})$, where $F_{\max}$ and $F_{\min}$ are the two extremes of the computed flux values. Whenever DUSTY calculates also the density profile η for spherical case, the numerical accuracy of that calculation is controlled by the same $q_{\rm acc}$.

The recommended flux accuracy value of 10% is entered in all the sample input files. The accuracy level that can be accomplished is related to the number of grid points and the model's overall optical depth. If the desired accuracy is not achieved, finer grids are generated automatically by DUSTY. The maximum number of grid points is bound by DUSTY's array dimensions, which are controlled by the parameter `npy` whose default value is 120. This internal limit suffices to ensure convergence at the 10% level for most models with $\tau_V \lesssim 1000$.[3] If higher levels of accuracy or larger τ_V are needed, DUSTY's internal limits on array sizes must be expanded by increasing `npy`, as described in §7.1.

4.6 Output Control

The final input entries control DUSTY's output. All output and its control is explained in the next section.

5 Output: Sphere

A typical DUSTY run generates an enormous amount of information, and the volume of output can easily get out of hand. To avoid that, DUSTY's default output is a single file that lists only minimal information about the run, as described next. All other output is optional and fully controlled by the user.

5.1 Default Output for Sphere

DUSTY always produces the output file `fname.out` for each model input `fname.inp`. In addition to a summary of the input parameters, the default output file tabulates global properties for each of the optical depths covered in the run.

The table's left column lists the sequential number `###` of the model with the fiducial optical depth `tau0` listed in the next column. Subsequent columns list quantities calculated by DUSTY for that `tau0`:

- ◇ `Psi/Psi0` – Psi as defined by eq.14 in IE97 with optically thin value Psi0= 6.06E+00
- ◇ `Fi` – the bolometric flux, in W m^{-2}, at the inner radius $y = 1$. Only the central source contributes to `Fi`; the diffuse flux vanishes at $y = 1$ under the point source assumption and the external radiation field carries no flux because it is isotropic. The bolometric flux emerging from the spherical distribution is `F1`$/Y^2$.

  Any measure of the shell dimension is irrelevant to the radiative transfer problem and thus not part of DUSTY's calculations. Still, the shell size can be of considerable interest in many

[3] Convergence and execution speed can be affected by the input radiation spectral shape. A hard spectrum heavily weighed toward short wavelengths, where the opacity is high, can have an effect similar to large τ_V.

applications. For convenience, the next three output items list different measures of the shell size expressed in terms of redundant quantities such as the luminosity:

◇ `r1(cm)` – the shell inner radius. If the heating radiation strength is specified through option `T1` (see §4.2.2) then `r1` is the radius where this is the dust temperature. This radius scales in proportion to $L^{1/2}$, where L is the luminosity. The tabulated value corresponds to $L = 10^4\ L_\odot$.

◇ `r1/rc` – where `rc` is the radius of the central source. This quantity scales in proportion to $(T_e/T_1)^2$, where T_e is the external radiation effective temperature. The listed value is for $T_e = 10,000$ K with two exceptions: when the spectral shape of the external radiation is the Planck or Engelke-Marengo function, the arguments of those functions are used for T_e.

◇ `theta1` – the angular size, in arcsec, of the shell inner diameter. This angle depends on the observer's position and scales in proportion to $F_{\rm obs}^{1/2}$, where $F_{\rm obs}$ is the observed bolometric flux. The tabulated value corresponds to $F_{\rm obs} = 10^{-6}$ W m^{-2}.

◇ `T1` – the dust temperature, in K, at the envelope's inner boundary. When the specified input radiation strength (see §4.2.2) produces a temperature in excess of the sublimation temperature `Tsub`, DUSTY will print a warning message.

◇ `Td` – the dust temperature, in K, at the envelope's outer boundary ($y = Y$).

◇ `RPr(1)` – The ratio of radiation pressure to gravitational force at the inner boundary. Both forces are per unit volume:

$$\frac{\mathcal{F}_{\rm rad}}{\mathcal{F}_{\rm grav}} = \frac{1}{4\pi G c m} \cdot \frac{L}{M} \cdot \frac{n_d \sigma_V}{n_H} \int Q_\lambda f_\lambda \, d\lambda \tag{5}$$

Here m is the mass of a hydrogen atom, $f_\lambda = F_\lambda / \int F_\lambda d\lambda$ is the local spectral shape, n_d the dust number density and n_H the number density of hydrogen nuclei. This expression holds only if the gas and dust are fully collisionally coupled. The tabulated value is for the standard Galactic value $n_d\sigma_V/n_H = 5 \cdot 10^{-22}$ cm^{-2} and for $L/M = 10^4\ L_\odot/M_\odot$.

◇ `err` – the numerical accuracy, in `%`, achieved in the run. Specifically, if r is the ratio of smallest to largest bolometric fluxes in the shell (after accounting for radial dilution in a centrally heated spherical shell), then the error is $(1-r)/(1+r)$. Errors smaller than 1% are listed as zero.

When the density distribution is derived from a hydrodynamics calculation for AGB winds (§4.1.2), three more columns are added to `fname.out`:

◇ `Mdot` – the mass loss rate in $M_\odot$ yr^{-1}. This quantity has $\sim 30\%$ inherent uncertainty because varying the gravitational correction from 0 up to 50% has no discernible effect on the observed spectrum.

◇ `Ve` – the terminal outflow velocity in km s^{-1}. The provided solutions apply only if this velocity exceeds 5 km s^{-1}. `Ve` is subject to the same inherent uncertainty as `Mdot`.

◇ `M>` – an upper limit in $M_\odot$ on the stellar mass M. The effect of gravity is negligible as long as M is less than 0.5`*M>` and the density profile is then practically independent of M.

These quantities posses general scaling properties in terms of the luminosity L, gas-to-dust mass ratio $r_{\rm gd}$ and dust grain bulk density ρ_s [3, 11]; the tabulations are for $L = 10^4\ L_\odot$, $r_{\rm gd} = 200$ and $\rho_s = 3$ g cm^{-3}. There is a slight complication with these tabulations when the dust optical properties are entered using `optical properties = 3` (§4.3.1). With this option, the scattering and absorption cross sections are entered in a file, tabulated using arbitrary units since only their spectral shape is relevant for the solution of the radiative transfer problem. However, the conversion to mass-loss rate requires also the grain size, and this quantity is not specified when `optical properties = 3` is used. DUSTY assumes that the entered values correspond to σ/V, the cross section per grain volume in μm^{-1}. If that is not the case, in the scaling relations $r_{\rm gd}$ must be replaced with $r_{\rm gd}V/\sigma$.

Finally, DUSTY assumes that the external radiation originates in a central point source. This assumption can be tested with eqs. (27) and (28) of [10] which give expressions for the central source angular size and occultation effect. From these it follows that the error introduced by the point-source assumption is no worse than 6% whenever

$$T_e > 2 \times \max[T_1, (F_{e1}/\sigma)^{1/4}] \tag{6}$$

where T_e is the effective temperature of the central source and F_{e1} is its flux at the shell inner boundary; note again that with the point source assumption, `F1` $= F_{e1}$. Thanks to scaling, T_e need not be specified and is entirely arbitrary as far as DUSTY is concerned. However, compliance with the point-source assumption implies that the output is meaningful only for sources whose effective temperature obeys eq. 6. For assistance with this requirement, `fname.out` lists the lower bound on T_e obtained from this relation for optically thin sources. Since F_{e1} decreases with optical depth when `T1` is specified as input (see [10]), the listed bound ensures compliance for all the models in the series. However, in optically thick cases F_{e1} may become so small that the listed bound will greatly exceed the actual limit from eq. 6. In those cases, the true bounds can be obtained, if desired, from eq. 6 and the model tabulated `F1`.

Black-body emission provides an absolute upper bound on the intensity of any thermal source. Therefore, input radiation whose spectral shape is the Planck function at temperature T is subject to the limit $T_e \le T$ even though T_e is arbitrary in principle. In such cases T must comply with eq. 6, otherwise DUSTY's output is suspect and in fact could be meaningless. DUSTY issues a stern warning after the tabulation line of any model with input spectral shape that is either the Planck or Engelke-Marengo function whose temperature violates eq. 6.

5.2 Optional Output for Sphere

In addition to the default output, the user can obtain numerous tabulations of spectra, imaging profiles and radial distributions of various quantities of interest for each of the optical depths included in the run. This additional output is controlled through flags entered at the end of the input file `fname.inp` that turn on and off the optional tabulations. Setting all flags to 0, as in `sphere1.inp` and `slab1.inp`, suppresses all optional tabulations and results in minimal output. A non-zero output flag triggers the production of corresponding output, occasionally requiring

additional input. Further user control is provided by the value of the output flag. When a certain flag is set to 1, the corresponding output is listed in a single file that contains the tabulations for all the optical depth solutions. Setting the flag to 2 splits the output, when appropriate, tabulating the solution for each optical depth in its own separate file. This may make it more convenient for plotting purposes, for example, at the price of many small files. A few flags can also be set to 3, splitting the output even further.

Each of the following subsections describes in detail the optional tabulations triggered by one of the output flags and any additional input it may require. Appendix A summarizes all the output flags and the corresponding output files they trigger, and can be used for quick reference.

5.2.1 Detailed spectra for each model

The next output flag triggers listing of detailed spectra for each model in the run. Setting this flag to 1 produces tables for the emerging spectra of all models in the single output file `fname.stb`. Setting the flag to 2 places each table in its own separate file, where file `fname.s###` contains the tabulation for model number `###` in the optical depth sequence listed in the default output file (§ 5.1).

Spectra are tabulated in terms of their spectral shapes $f(\lambda) = \lambda F_\lambda / \int F_\lambda d\lambda$, where F_λ is the relevant flux. The corresponding scale $F = \int F_\lambda d\lambda$ in [W/m^2] is listed in the table's first row (specified with a wavelength of -1), followed by listing of f_λ. Values smaller than 10^{-20} are listed as 0. In addition to the emerging spectrum, the table for each model also lists separately the contributions of various components to the overall flux, the spectral shape of the input radiation, and the wavelength dependence of the total optical depth. The tabulated quantities are :

- ◇ `lambda` – the wavelength in μm
- ◇ `fTot` – the spectral shape of the total emerging flux
- ◇ `xAtt` – fractional contribution of the attenuated input radiation to `fTot`
- ◇ `xDs` – fractional contribution of the scattered radiation to `fTot`
- ◇ `xDe` – fractional contribution of the dust emission to `fTot`
- ◇ `fInp` – the spectral shape of the input (unattenuated) radiation
- ◇ `tauT` – overall optical depth at wavelength `lambda`
- ◇ `albedo` – the albedo at wavelength `lambda`

5.2.2 Images at specified wavelengths

The surface brightness is a luminosity-independent self-similar distribution [8] of b/r_1, the impact parameter scaled by the envelope inner radius (fig. 2); note that r_1 is listed in the default output file (§5.1) for a source luminosity $10^4\ L_\odot$. DUSTY can produce maps of the surface brightness at up to 20 wavelengths, specified in the input file. Setting the option flag to 1 produces imaging

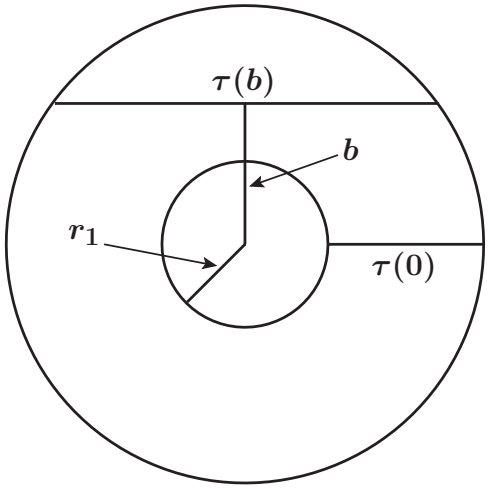

Figure 2: Notation for imaging output.

tabulations for all the models of the run in the single output file `fname.itb`, setting the flag to 2 puts the table for model number `###` in its separate file `fname.i###`.

Following the option selection flag, the number (≤ 20) of desired wavelengths is entered first, followed by a list of these wavelengths in μm.

- Example of additional input data required in `fname.inp` for imaging output:

```
imaging tables (all models in one file) = 1
number of wavelengths = 8
wavelengths = 0.55, 1.0, 2.2, 4, 10, 50, 100, 1000  micron
```

Whenever a specified wavelength is not part of DUSTY's grid, the corresponding image is obtained by linear interpolation from the neighboring wavelengths in the grid. If the nearest wavelengths are not sufficiently close, the interpolation errors can be substantial. For accurate modeling, all wavelengths specified for imaging should be part of the grid, modifying it if necessary (see §7.2).

Each map is tabulated with a single header line as follows:

- ◇ `b` $= b/r_1$, where b is the impact parameter.
- ◇ `t(b)` $= \tau($`b`$)/\tau($`0`$)$, where $\tau($`b`$)$ is the overall optical depth along a path with impact parameter `b`. Note that $\tau(0)$ is simply the overall radial optical depth `tauT`, listed in the file `fname.s###` (§5.2.1), and that `t(b)` doubles its value across the shell once the impact parameter exceeds the stellar radius.
- ◇ The intensity, in Jy arcsec^{-2}, at each of the wavelengths listed in the header line.

A typical image contains a narrow central spike of width $b_c = 2r_c/r_1$, where r_c is the radius of the central source [8]. Since this feature is unresolved in most observations, it is usually of limited interest. This spike is the only feature of the emerging intensity that depends on the

effective temperature T_e of the central source, which is irrelevant to DUSTY's calculations. The width of the spike scales in proportion to T_e^{-2}, its height in proportion to T_e^4. The listed value is for $T_e = 10,000$ K with two exceptions: when the spectral shape of the external radiation is the Planck or Engelke-Marengo function, the arguments of those functions are used for T_e.

5.2.3 Radial profiles for each model

The next option flag triggers tabulations of the radial profiles of the density, optical depth and dust temperature. Setting the flag to 1 produces tabulations for all the models of the run in the single output file `fname.rtb`, setting the flag to 2 places the table for model number `###` in its own separate file `fname.r###`. The tabulated quantities are:

- ◇ `y` – dimensionless radius
- ◇ `eta` – the dimensionless, normalized radial density profile (§4.1.1)
- ◇ `t` – radial profile of the optical depth variation. At any wavelength λ, the optical depth at radius y measured from the inner boundary is `t*tauT`, where `tauT` is the overall optical depth at that wavelength, tabulated in the file `fname.s###` (§5.2.1).
- ◇ `tauF` – radial profile of the flux-averaged optical depth
- ◇ `epsilon` – the fraction of grain heating due to the contribution of the envelope to the radiation field (see [10]).
- ◇ `RPr` – radial profile of the ratio of radiation pressure to gravitational force normalized to the value of the ratio at the inner boundary, `RPr`$(y = 1)$. The inner boundary value is listed in the default file `fname.out` (§5.1).
- ◇ `Td` – radial profile of the dust temperature

The radial profiles `eta`(y) and `t`(y) determine also the radial runs of gas density and column density once a dust-to-gas ratio is assumed; the standard conversion is that the hydrogen column associated with dust optical depth τ_V is $N_{\rm H} = 2 \cdot 10^{21}\ \tau_V$ cm^{-2}. Then the radial profiles of gas column and volume densities are

$$N_{\rm H}(y) = N_{\rm H} \times \texttt{t}(y), \qquad n_{\rm H}(y) = (N_{\rm H}/r_1) \times \texttt{eta}(y) \tag{7}$$

In the case of dynamical calculation with `density type = 3` for AGB stars (§4.1.2), the following additional profiles are tabulated:

- ◇ `u` – the dimensionless radial velocity profile normalized to the terminal velocity `Ve`, which is tabulated for the corresponding overall optical depth in file `fname.out` (§5.1).
- ◇ `drift` – the radial variation of $v_{\rm g}/v_{\rm d}$, the velocity ratio of the gas and dust components of the envelope. This quantity measures the relative decrease in dust opacity due to dust drift.

5.2.4 Detailed Run-time messages

In case of an error, the default output file issues a warning. Optionally, additional, more detailed run-time error messages can be produced and might prove useful in tracing the program's progress in case of a failure. Setting the corresponding flag to 1 produces messages for all the models in the single output file `fname.mtb`, setting the flag to 2 puts the messages for model number `###` in its own separate file `fname.m###`.

6 Output: Slab

6.1 Default Output for Slab

DUSTY always produces the output file `fname.out` for each model input `fname.inp`. In addition to a summary of the input parameters, the default output file tabulates global properties for each of the optical depths covered in the run.

The table's left column lists the sequential number `###` of the model with the fiducial optical depth `tau0` listed in the next column. Subsequent columns list quantities calculated by DUSTY for that `tau0`:

- ◇ `Psi/Psi0` – Psi as defined by eq.14 in IE97 with optically thin value Psi0= 4.78E+01
- ◇ `FiL` – input bolometric flux, in $\mathrm{W\,m^{-2}}$, of the left-side source at the slab left boundary.
- ◇ `FiR` – input bolometric flux, in $\mathrm{W\,m^{-2}}$, of the right-side source at the slab left boundary.
- ◇ `FbolL` – bolometric flux, in $\mathrm{W\,m^{-2}}$, at the left slab boundary.
- ◇ `FbolR` – bolometric flux, in $\mathrm{W\,m^{-2}}$, at the right slab boundary.
- ◇ `r1(cm)` – the distance at which a point source with luminosity $10^4\ L_\odot$ produces the bolometric flux F_{e1}.
- ◇ `TdL(K)` – the dust temperature at the slab left boundary. When the specified input radiation strength (see §4.2.2) produces a temperature in excess of the sublimation temperature `Tsub`, DUSTY will print a warning message.
- ◇ `TdR(K)` – the dust temperature at the slab right boundary. See previous item for values in excess of `Tsub`.
- ◇ `RPr(1)` – The ratio of radiation pressure to gravitational force at the left boundary. Both forces are per unit volume:

$$\frac{\mathcal{F}_{\rm rad}}{\mathcal{F}_{\rm grav}} = \frac{1}{4\pi G c m} \cdot \frac{L}{M} \cdot \frac{n_d \sigma_V}{n_H} \int Q_\lambda f_\lambda \, d\lambda \tag{8}$$

Here m is the mass of a hydrogen atom, $f_\lambda = F_\lambda / \int F_\lambda d\lambda$ is the local spectral shape, n_d the dust number density and n_H the number density of hydrogen nuclei. This expression holds only if the gas and dust are fully collisionally coupled. The tabulated value is for the standard Galactic ratio $n_d \sigma_V / n_H = 5 \cdot 10^{-22}$ cm^{-2} and for $L/M = 10^4\ L_\odot / M_\odot$.

◇ `err` – the flux conservation error, defined as in the spherical case.

DUSTY's distribution contains three sample input files, `slab1.inp`, `slab2.inp` and `slab3.inp`, which can be used as templates for the slab geometry. The output generated with `slab1.inp` is shown in appendix D.

6.2 Optional Output for Slab

6.2.1 Detailed spectra for each model

The next output flag triggers listing of detailed spectra for each model in the run. Setting this flag to 1 producerrs tables for the emerging spectra of all models in the single output file `fname.stb`. Setting the flag to 2 places each table in its own separate file, where file `fname.s###` contains the tabulation for model number `###` in the optical depth sequence listed in the default output file (§6.1).

The structure of the output is the same as for the sphere (Sect. 5.2.1). Spectra are tabulated in terms of their spectral shapes $f(\lambda) = \lambda F_\lambda / \int F_\lambda d\lambda$, where F_λ is the relevant flux. The corresponding scale $F = \int F_\lambda d\lambda$ in [W/m^2] is listed in the table's first row (specified with a wavelength of -1), followed by listing of f_λ. Values smaller than 10^{-20} are listed as 0. In addition to the emerging spectrum, the table for each model also lists separately the contributions of various components to the overall flux, the spectral shape of the input radiation, and the wavelength dependence of the total optical depth. The tabulated quantities are :

◇ `lambda` – the wavelength in μm

◇ `fRight/fLeft` – the spectral shape of the total flux emerging from the right/left side of the slab.

◇ `xAtt` – fractional contribution of the attenuated input radiation to `fTot`

◇ `xDs` – fractional contribution of the scattered radiation to `fTot`

◇ `xDe` – fractional contribution of the dust emission to `fTot`

◇ `fInp_L/fInp_R` – the spectral shape of the input (unattenuated) radiation from left/right side of the slab

◇ `tauT` – overall optical depth at wavelength `lambda`

◇ `albedo` – the albedo at wavelength `lambda`

6.2.2 Intensities for each model

The next output flag triggers listing of the intensity for user specified angles for each model in the run. Setting this flag to 1 produces tables for the emerging spectra of all models in the single output file `fname.itb`. Setting the flag to 2 places each table in its own separate file, where file

`fname.i###` contains the tabulation for model number `###` in the optical depth sequence listed in the default output file (§6.1).

After triggering the the intensities file with the output flag the angle grid has to be specified. First the type of the grid either linear (1) or logarithmic (2). The next input is the minimum angle followed by the maximum angle and the steppsize inbetween.

```
intensities at specified angles;     fname.i### = 2
angletype = 1 (linear)
theta_min = 0 theta_max = 80 stepp = 5
```

The tabulated quantities are :

- ◇ `lambda` – the wavelength in μm
- ◇ `angle` – the transmitted Intensity as $I(\theta)cos(\theta)$ in [W/sr]

6.2.3 Spatial Profiles

The output for spatial profiles is similar to the spherical case. The radial distance `y` and density profile `eta` are removed. The relative distance in optical depth from the left boundary, `t`, becomes the running variable, and the tabulations of `tauF`, `epsilon`, `Td` and `RPr` are the same (see 5.2.3).

6.2.4 Detailed Run-time messages

These messages are triggered in the same way as in the spherical case (see §5.2.4).

7 User Control of DUSTY

DUSTY allows the user control of some of its inner working through tinkering with actual code statements that control the spatial and spectral grids. The appropriate statements were placed in the file `userpar.inc` separate from the main `dusty.f`, and are imbedded during compilation by the FORTRAN statement `INCLUDE`; note that `userpar.inc` *must always stay with the source code in the same directory.* After modifying statements in `userpar.inc` , DUSTY must be recompiled to enable the changes.

7.1 Array Sizes for Spatial Grid

The maximum size of DUSTY's spatial grid is bound by array dimensions. These are controlled by the parameter `npY` which sets the limit on the number of radial points. The default value of 40 must be decreased when DUSTY is run on machines that lack sufficient memory (see §1) and increased when DUSTY fails to achieve the prescribed accuracy (see §4.5). This parameter is defined in `userpar.inc` via

```
PARAMETER (npY=512)
```

To modify `npY` simply open `userpar.inc`, change the number 40 to the desired value, save your change and recompile. That's all. Every other modification follows a similar procedure. Since DUSTY's memory requirements vary roughly as the second power of `npY`, the maximum value that can be accommodated on any given machine is determined by the system memory.

The parameter `npY` defines also the size `npP` of the grid used in angular integrations. In the case of planar geometry DUSTY uses analytic expressions for these integrations. Since this grid becomes redundant, `npP` can be set to unity, allowing a larger maximum `npY`. The procedure is described in `userpar.inc`.

7.2 Wavelength Grid

DUSTY's wavelength grid is used both in the internal calculations and for the output of all wavelength dependent quantities. The number of grid points is set in `userpar.inc` by the parameter `npL`. The grid itself is read from the file `lambda_grid.dat`, which *must always stay in the directory* `data`. This file starts with an arbitrary number of header lines, the beginning of the wavelength list is signaled by an entry for the number of grid points. This number must be equal to `npL` entered in `userpar.inc` and to the actual number of entries in the list.

The grid supplied with DUSTY contains 125 points from 0.01 to 3.6×10^4 μm. The short wavelength boundary is to ensure adequate coverage of input radiation from an O star, for example, which peaks at 0.1 μm. Potential effects on the grain material by such hard radiation are not included in DUSTY. The long wavelength end is to ensure adequate coverage at all wavelengths where dust emission is potentially significant. Wavelengths can be added and removed provided the following rules are obeyed:

- Wavelengths are specified in μm.
- The shortest wavelength must be 0.01 μm, the longest 3.6×10^4 μm.
- The ratio of each consecutive pair must be ≤ 1.5.

The order of entries is arbitrary, DUSTY sorts them in increasing wavelength and the sorted list is used for all internal calculations and output. This provides a simple, convenient method for increasing the resolution at selected spectral regions: just add points at the end of the supplied grid until the desired resolution is attained. Make sure you update both entries of `npL` and recompile DUSTY.

In practice, tinkering with the wavelength grid should be reserved for adding spectral features. Specifying the optical properties of the grains at a resolution coarser than that of the wavelength grid defeats the purpose of adding grid points. The optical properties of grains supported by DUSTY are listed on the default wavelength grid. Therefore, modeling of very narrow features requires both the entry of a finer grid in `lambda_grid.dat` and the input of user-supplied optical properties (see §4.3.1) defined on that same grid.

Appendices

A Output Summary

DUSTY's default output is the file `fname.out`, described in §5.1 (sphere) and §6.1 (slab). Additional output is optionally produced through selection flags, summarized in the following table. The second column lists the section number where a detailed description of the corresponding output is provided.

Table 1: Summary of all Output Options

Output Listing	§	Output File Triggered by Flag		
		1	2	3
Sphere				
Detailed spectra, each model	5.2.1	`fname.stb`	`fname.s###`	`fname.s###`
Images	5.2.2	`fname.itb`	`fname.i###`	`fname.i###`
Radial profiles	5.2.3	`fname.rtb`	`fname.r###`	
Error messages	5.2.4	`fname.mtb`	`fname.m###`	
Slab				
Detailed spectra, each model	6.2.1	`fname.stb`	`fname.s###`	`fname.s###`
Intensities	6.2.2	`fname.itb`	`fname.i###`	`fname.i###`
Spatial profiles	6.2.3	`fname.rtb`	`fname.r###`	
Error messages	6.2.4	`fname.mtb`	`fname.m###`	

B Pitfalls, Real and Imaginary

This appendix provides a central depository of potential programming and numerical problems. Some were already mentioned in the text and are repeated here for completeness.

- FORTRAN requires termination of input records with a carriage return. Make sure you press the "Enter" key whenever you enter a filename in the last line of `dusty.mas`.
- In preparing input files, the following two rules must be carefully observed: (1) all required input entries must be specified, and in the correct order; (2) the equal sign, '=', must be entered only as a flag to numerical input. When either rule is violated and DUSTY reaches the end of the input file while looking for additional input, you will obtain the error message:

```
****TERMINATED. EOF reached by RDINP while looking for input.
*** Last line read:
```

This message is a clear sign that the input is out of order.

- On occasion, when the execution results in a segmentation fault under Linux or MacOS, increasing the stacksize of the console may solve the problem. This can be done as follows:

  for a bash shell: `ulimit -s unlimited`
  for a tcsh shell: `limit stacksize unlimited`

C Sample Output File: sphere1.out

```
 ============================
  Output from program dusty
  version: 4.00
 ============================

  Input parameters from file:
  examples/sphere1/sphere1.inp
* ------------------------------------------------------------------------
* NOTES:
* Sample input file (sphere1.inp)
* Spherical dust distribution with
* constant density profile
* heated by external radiation with a Black Body of 5000K
* for composite dust grain 70% silicates 30% carbon
* for 3 optical depth (30,40,50)
* ------------------------------------------------------------------------
  Central source spectrum described by
   a single Black Body with temperature     5800.00 K
  Dust temperature on the inner boundary:   0.0000000000000000       K
  ------------------------------------------
  density described by 1/r**k with k =  0.0
  relative thickness: 1.000E+03
  ------------------------------------------
  Optical depth at 5.5E-01 microns: 1.00E+01
   Required Flux accuracy:       10.00%
   Required Temp accuracy:        0.24%
  ------------------------------------------
  ------------------------------------------

  RESULTS:
  --------
 ###   tau0   Psi/Psi0 Fi(W/m2)  r1(cm)   r1/rc    theta1   T1(K)    Td(K)    RPr(1)  e(%)
 ###     1       2        3        4        5        6        7        8        9      10
 ================================================================================================
   1 1.00E+01 1.01E+00 7.70E+04 1.99E+14 2.89E+01 1.49E+00 1.20E+03 4.81E+01 1.39E+07   2
 ====================================
  (1) optical depth at 5.5E-01 microns
  (2) Psi as defined by eq.14 in IE97 with optically thin value Psi0= 6.06E+00
  (3) bolometric flux at the inner radius
  (4) inner radius for L = 1e4 Lo
  (5) ratio of the inner to the stellar radius
  (6) angular size (in arcsec) when Fbol=1e-6 W/m2
```

```
  (7) dust temperature at the inner radius
  (8) dust temperature at the outer edge
  (9) radiation pressure on inner boundary; see manual for units
 (10) maximum error in flux conservation (Fmax-Fmin)/(Fmax+Fmin)
 ================================================
 Everything is ok for all models.
 Spectra are in files *.s##
 Radial profiles are in files *.r##
 Run-time messages are in files *.m##
 ========== the end ============================
```

D Sample Output File: `slab1.out`

```
 ===========================
  Output from program dusty
  version: 4.00
 ===========================

  Input parameters from file:
  examples/slab1/slab1.inp
* ------------------------------------------------------------------------
* NOTES:
* Sample input file (slab1.inp)
* directional input of power law spectrum
* left side temperature of 800 K
* ------------------------------------------------------------------------

  Left-side source spectrum described by
    Power law with:
     lambda      k
  1.000E-02
            0.000E+00
  1.000E-01
            5.000E-01
  1.000E+00
            3.000E+00
  3.600E+04
  Dust temperature on the inner boundary:   1200.0000000000000       K
  Calculation in planar geometry:
  Directional illumination from the left.
  ----------------------------------------
  Optical depths at 5.5E-01 microns
```

```
 ranging from 1.00E+01 to 2.00E+01
   2 models with grid from file
   examples/slab1/tauV.tab
  Required Flux accuracy:        5.00%
  Required Temp accuracy:        0.12%
 -----------------------------------------
 Intensity requested for these theta_out(deg):
    0.0    5.0   10.0   15.0   20.0   25.0   30.0   35.0
   40.0   45.0   50.0   55.0   60.0   65.0   70.0   75.0
   80.0
  equidistant in theta_out, step= 5.0
 -----------------------------------------

 RESULTS:
 --------
###    Tau0    Psi/Psi0     FiL      FiR       FbolL    FbolR     r1(cm)    TdL(K)    TdR(K)
###      1        2          3        4          5        6         7          8         9
=================================================================================================
  1  1.00E+01  1.53E+00  6.97E+02  0.00E+00 -7.04E+03  7.01E+03  2.09E+15  8.00E+02  7.04E+02
  2  2.00E+01       NaN       NaN       NaN       NaN       NaN       NaN       NaN       NaN
====================================
 (1) optical depth at 5.5E-01 microns
 (2) Psi as defined by eq.14 in IE97 with optically thin value Psi0=      NaN
 (3) input bol.flux (in W/m2) of the left-side source at the left slab boundary
 (4) input bol.flux (in W/m2) of the right-side source at the right slab boundary
 (5) bolometric flux (in W/m2) at the left slab boundary
 (6) bolometric flux (in W/m2) at the right slab boundary
 (7) position of the left slab boundary for L = 1e4 Lo
 (8) dust temperature at the left slab boundary
 (9) dust temperature at the right slab boundary
 (10) radiation pressure on left boundary; see manual for units
 (11) maximum error in flux conservation (Fmax-Fmin)/(Fmax+Fmin)
 ================================================
 Everything is ok for all models.
 Spectra are in files *.s##
 Intensities are in files *.i##
 Radial profiles are in files *.r##
 Run-time messages are in files *.m##
========== the end ============================
```

E Library of Optical Constants

DUSTY's distribution includes a library of data files with the complex refractive indices of various compounds of interest. The files are standardized in the format DUSTY accepts. Included are the optical constants for the seven built-in dust types as well as other frequently encountered astronomical dust components. This library will be updated continuously at the DUSTY site. The following table lists all the files currently supplied.

Table 2: Optical Constants Library Supplied with Dusty

File Name	Compound	Range (μm)	Ref
`Al2O3-comp.nk`	Al_2O_3-compact	7.8 – 200	[13]
`Al2O3-por.nk`	Al_2O_3-porous	7.8 – 500	[13]
`amC-hann.nk`	amorphous carbon	0.04 – 905	[5]
`amC-zb1.nk`	amorphous carbon (BE)	0.05 – 1984	[22]
`amC-zb2.nk`	amorphous carbon (ACAR)	0.04 – 1984	[22]
`amC-zb3.nk`	amorphous carbon (ACH2)	0.04 – 948	[22]
`crbr300.nk`	crystalline bronzite	6.7 – 487.4	[6]
`crMgFeSil.nk`	crystalline silicate	6.7 – 584.9	[13]
`FeO.nk`	FeO (5.7g/ccm)	0.2 – 500	[13]
`gloliMg50.nk`	glassy olivine	0.2 – 500	[1]
`glpyr300.nk`	glassy pyroxene at 300 K	6.7 – 487	[6]
`glpyrMg50.nk`	glassy pyroxene	0.2 – 500	[1]
`glSil.nk`	glassy silicate	0.4 – 500	[12]
`grph1-dl.nk`	graphite, $E \perp c$	0.001 – 10^3	[2]
`grph2-dl.nk`	graphite, $E \parallel c$	0.001 – 10^3	[2]
`opyr-pwd.nk`	ortho-pyroxenes - powder	5.0 – 25	[20]
`opyr-slb.nk`	ortho-pyroxenes - slab	5.0 – 25	[20]
`OssOdef.nk`	O-deficient CS silicate	0.4 – 10^4	[18]
`OssOrich.nk`	O-rich IS silicate	0.4 – 10^4	[18]
`SiC-peg.nk`	α-SiC	0.03 – 2000	[19]
`Sil-dlee.nk`	"Astronomical silicate"	0.03 – 2000	[2]
`Sil-oss1.nk`	warm O-deficient silicates	0.4 – 10^4	[18]
`Sil-oss2.nk`	cold O-rich silicate	0.4 – 10^4	[18]

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