Explanation of the size distributions

In the database we provide tables for the size distributions $S(\log r)$, $N(\log r)$, and $V(\log r)$. The main purpose of the text below is to provide definitions and interrelations for these size distributions. We note that we have tabulated $S(\log r)$, $N(\log r)$, and $V(\log r)$ in the database by numbers consisting of three figures to avoid rounding errors to accumulate in calculations involving these functions, even though the actual uncertainties of these functions are not known.

1 Number distributions

Consider a collection of randomly oriented particles with arbitrary shapes. Replace each particle by a sphere having the same average (over all orientations) projected surface area. This creates a collection of spheres which we shall call projected-surface-equivalent spheres, or briefly spheres. Let $r$ denote the radius of such a sphere. We introduce a function $\nu(r)$ so that $\nu(r)\,dr$ is the number of spheres per unit volume (of space) having radii between $r$ and $r + \,dr$. Thus, the number of spheres per unit volume with radii between between $r_1$ and $r_2$ is given by $\int_{r_1}^{r_2} \nu(r)\,dr$. Units of $\nu(r)$ are, e.g., $\mu$m$^{-1}$cm$^{-3}$.

The total number of spheres per unit volume is

$$N = \int_0^\infty \nu(r)\,dr. \quad (1)$$

Units of $N$ are for example cm$^{-3}$. We shall call $\nu(r)$ a number distribution (function) and

$$n(r) = \nu(r)/N. \quad (2)$$

a normalized number distribution of the collection of particles. Units for the latter are, e.g., $\mu$m$^{-1}$. Hence $n(r)\,dr$ is the fraction of the total number of particles per unit volume having radii between $r$ and $r + \,dr$. Consequently, the relative contribution of spheres with radii between $r_1$ and $r_2$ to the total number of particles per unit volume can be written as

$$\frac{\int_{r_1}^{r_2} \nu(r)\,dr}{N} = \int_{r_1}^{r_2} n(r)\,dr. \quad (3)$$
Note that this quantity is dimensionless and can be expressed in percent.

Obviously, we have

\[ \int_0^\infty n(r) \, dr = 1, \]  

(4)

which, in practice, gives a handy test for a normalized number distribution \( n(r) \).

2 Volume distributions

The total volume occupied by the (projected-surface-area-equivalent) spheres per unit volume of space is

\[ V = \int_0^\infty \nu(r) \left( \frac{4}{3} \pi r^3 \right) \, dr. \]  

(5)

Units of \( V \) are, e.g., \( \mu m^3 cm^{-3} \). The relative contribution to this by spheres with radii between \( r_1 \) and \( r_2 \) is dimensionless and given by \( \int_{r_1}^{r_2} \nu(r) \, dr \), where the normalized volume distribution of the collection of particles

\[ v(r) = \frac{\nu(r) \frac{4}{3} \pi r^3}{V}. \]  

(6)

Units of \( v(r) \) are, e.g., \( \mu m^{-1} \). A handy test is provided by

\[ \int_0^\infty v(r) \, dr = 1. \]  

(7)

3 Projected-surface-area distributions

We can define projected-surface-area distributions analogous to volume distributions. Thus, the relative contribution to the total surface area of projected-surface-area-equivalent spheres with radii between \( r_1 \) and \( r_2 \) per unit volume of space is the dimensionless quantity

\[ \frac{\int_{r_1}^{r_2} \nu(r) \pi r^2 \, dr}{\int_0^\infty \nu(r) \pi r^2 \, dr} = \frac{\int_{r_1}^{r_2} \nu(r) \pi r^2 \, dr}{S} = \int_{r_1}^{r_2} s(r) \, dr, \]  

(8)
where $S$ (in units of, for instance, $\mu m^2\text{cm}^{-3}$) is the total projected surface area occupied by the spheres per unit volume of space and the normalized projected-surface-area distribution of the collection of particles

$$
    s(r) = \frac{\nu(r) \pi r^2}{S} = \frac{\nu(r) r^2}{\int_0^\infty \nu(r) r^2 \, dr}.
$$

Units of $s(r)$ are, e.g., $\mu m^{-1}$. A handy test is provided by

$$
\int_0^\infty s(r) \, dr = 1.
$$

Note that all three functions $n(r)$, $v(r)$, and $s(r)$ are normalized size distributions of a particular collection of arbitrary particles in random orientation.

4 Interrelations for the size distributions

According to Eqs. (2),(6) and (9) we have the normalized number distribution

$$
    n(r) = \frac{\nu(r)}{N},
$$

the normalized volume distribution

$$
    v(r) = c_1 r^3 n(r), \quad \text{with} \quad c_1 = \frac{4}{3} \pi \frac{N}{V},
$$

and the normalized projected-surface-area distribution

$$
    s(r) = c_2 r^2 n(r), \quad \text{with} \quad c_2 = \frac{\pi}{S}.
$$

If one of the functions $n(r)$, $v(r)$, or $s(r)$ is given we can find the other two from Eqs. (11),(12), and (13) apart from constants, but these constants can be found directly from the normalization conditions expressed by Eqs. (4),(7), and (10). In studies of light scattering, the projected surface area is very important. Therefore, the so-called effective radius is often used (1). This is given by

$$
    r_{\text{eff}} = \frac{\int_0^\infty \nu \pi r^2 n(r) \, dr}{\int_0^\infty \nu r^2 n(r) \, dr} = \frac{3V}{4S} = \int_0^\infty r s(r) \, dr,
$$
which shows that \( s(r) \) is the weighting function here. To characterize size distributions with a few parameters, this effective radius and the effective standard deviation or the effective variance can conveniently be used. The effective standard deviation is defined as

\[
\sigma_{\text{eff}} = \sqrt{\frac{\int_0^\infty (r - r_{\text{eff}})^2 \pi r^2 n(r) \, dr}{\int_0^\infty \pi r^2 n(r) \, dr}} = \sqrt{\frac{\int_0^\infty (r - r_{\text{eff}})^2 s(r) \, dr}{r_{\text{eff}}^2 \int_0^\infty s(r) \, dr}}.
\] (15)

The effective variance \( v_{\text{eff}} \) equals \( \sigma_{\text{eff}}^2 \). When the sizes of the particles are considered relative to the wavelength \( \lambda \) of the scattered light the effective size parameter \( x_{\text{eff}} = 2\pi r_{\text{eff}} / \lambda \) can be employed. However, values for the effective radius and the effective standard deviation may be misleading if the size distribution is, for example, bimodal. In such a case other or more parameters are needed to describe the size distributions in a satisfactory way.

5 Plots

In plots we may like to use \( \log r \) where \( r \) is expressed in micrometers instead of \( r \) as the abscissa, especially when the range of \( r \) is very large. As an example we consider \( n(r) \). If we plot \( n(r) \) versus \( \log r \) we loose the simple interpretation of areas under the curve as relative number of particles in a certain size range (see Eq. (3)). But we can change the variable and define a new function \( N(\log r) \) so that \( N(\log r) \, d\log r \) is the relative number of spheres per unit volume (of space) in the size range \( \log r \) to \( \log r + d\log r \). So

\[
\int_{\log r_1}^{\log r_2} n(r) \, dr = \int_{\log r_1}^{\log r_2} N(\log r) \, d\log r = \int_{r_1}^{r_2} [N(\log r) \frac{d\log r}{dr}] \, dr = \int_{r_1}^{r_2} \frac{N(\log r)}{r \ln 10} \, dr
\] (16)

where \( \ln 10 \) is the natural logarithm of 10. Consequently

\[
N(\log r) = \ln 10 rn(r) = 2.303rn(r).
\] (17)

Eq. (16) shows that it is advantageous to plot \( N(\log r) \) versus \( \log r \) or in other words \( \ln 10rn(r) \) versus \( \log r \), because we can use the area rule again, i.e., equal areas under parts of the curve means equal relative amounts of spheres per unit volume in the ranges considered. In the literature cumulative size distributions, such as the cumulative number distribution \( n_c(r) \), are frequently encountered. Here \( n_c(r) \) is the fraction of particles per unit volume with radii smaller than \( r \), i.e., \( n_c(r) = \int_r^\infty n(r') \, dr' \) yielding for use in plots

\[
\frac{dn_c(r)}{d\log r} = \ln 10rn(r) = N(\log r).
\] (18)
So far we have considered \( n(r) \), but we can do the same for all absolute or relative (normalized) distribution functions (see Facts and Figures). Thus, we define

\[
S(\log r) = \ln 10rs(r) = 2.303rs(r)
\]

\[
V(\log r) = \ln 10rv(r) = 2.303rv(r).
\]

(19)

(20)

It should be noted that \( N(\log r) \), \( S(\log r) \), and \( V(\log r) \) are dimensionless functions which are also called size distributions. For normalized distributions one often omits the factor 2.303 and performs the normalization by integration of the resulting curve over the entire range (the total area under the curve).

A useful relation, that follows from using Eqs. (12)-(14) and Eqs. (19)-(20) is

\[
\frac{S(\log r)}{V(\log r)} = \frac{s(r)}{v(r)} = \frac{c_2}{c_1r} = \frac{r_{\text{eff}}}{r}.
\]

(21)

Thus, \( s(r_{\text{eff}}) = v(r_{\text{eff}}) \) and \( S(\log r_{\text{eff}}) = V(\log r_{\text{eff}}) \). For this reason the curves for \( S(\log r) \) and \( V(\log r) \) plotted versus \( \log r \) intersect at \( \log r_{\text{eff}} \). Consequently, \( r_{\text{eff}} \) can be quickly estimated from figures (see Facts and Figures) or tables like in the database. Furthermore, we have \( S(\log r) > V(\log r) \) if \( \log r < \log r_{\text{eff}} \) and \( S(\log r) < V(\log r) \) if \( \log r > \log r_{\text{eff}} \).

Similarly, Eq. (13) gives in combination with Eqs. (17) and (19)

\[
\frac{N(\log r)}{S(\log r)} = \frac{n(r)}{s(r)} = \frac{1}{c_2r^2} = \frac{S}{\pi N r^2}.
\]

(22)

So the curves for \( N(\log r) \) and \( S(\log r) \) intersect at \( \log r = \log \sqrt{\frac{S}{\pi N}} \) and \( N(\log r) > S(\log r) \) if \( \log r < \log \sqrt{\frac{S}{\pi N}} \) and \( N(\log r) < S(\log r) \) if \( \log r > \log \sqrt{\frac{S}{\pi N}} \).

References