AN INTERACTIVE PROGRAM FOR ESTIMATING EXTINCTION AND SCATTERING PROPERTIES OF MOST PARTICULATE CLOUDS

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B.T.N. Evans

ABSTRACT

An interactive computer program is described that enables the user to
calculate the phase function, extinction, scattering and absorption efficiencies, the mass
extinction coefficient and backscatter to extinction ratio for most particulate clouds.
These clouds may be composed of either mono- or polydispersed particles of the
following geometries: sphere, coated sphere, infinite cylinder, coated infinite cylinder,
finite cylinder or various irregular shapes. The non-spherical regular shapes may be
either oriented or have random orientation.
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<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>projected area of particle</td>
</tr>
<tr>
<td>$a$</td>
<td>parameter of Gates-Gaudin-Schumann size distribution</td>
</tr>
<tr>
<td>$b$</td>
<td>empirical parameter in modified gamma size distribution</td>
</tr>
<tr>
<td>$b$</td>
<td>width of Rosin-Rammler size distribution</td>
</tr>
<tr>
<td>$C$</td>
<td>mass concentration of aerosol</td>
</tr>
<tr>
<td>$C_{\text{abs}}$</td>
<td>absorption cross section</td>
</tr>
<tr>
<td>$C_{\text{ext}}$</td>
<td>extinction cross section</td>
</tr>
<tr>
<td>$C_{\text{sca}}$</td>
<td>scattering cross section</td>
</tr>
<tr>
<td>$F$</td>
<td>fraction of particles in non-Mie size regime</td>
</tr>
<tr>
<td>$F(x)$</td>
<td>particle size distribution</td>
</tr>
<tr>
<td>$I$</td>
<td>attenuated intensity of radiation</td>
</tr>
<tr>
<td>$I_0$</td>
<td>incident intensity of incoming radiation</td>
</tr>
<tr>
<td>$k$</td>
<td>imaginary part of index of refraction</td>
</tr>
<tr>
<td>$L$</td>
<td>distance through aerosol</td>
</tr>
<tr>
<td>$L$</td>
<td>length size parameter of finite fibre or cylinder</td>
</tr>
<tr>
<td>$l$</td>
<td>length of finite fibre or cylinder</td>
</tr>
<tr>
<td>$M$</td>
<td>mass of particle</td>
</tr>
<tr>
<td>$m$</td>
<td>index of refraction</td>
</tr>
<tr>
<td>$m_{\text{rel}}$</td>
<td>relative index of refraction</td>
</tr>
<tr>
<td>$m_1$</td>
<td>core index of refraction</td>
</tr>
<tr>
<td>$m_2$</td>
<td>coat index of refraction</td>
</tr>
<tr>
<td>$m_i$</td>
<td>either core or coat index of refraction</td>
</tr>
<tr>
<td>$n$</td>
<td>real part of index of refraction</td>
</tr>
<tr>
<td>$n$</td>
<td>parameter in Rosin-Rammler particle size distribution</td>
</tr>
<tr>
<td>$p$</td>
<td>phase function</td>
</tr>
<tr>
<td>$Q_{\text{abs}}$</td>
<td>absorption efficiency</td>
</tr>
<tr>
<td>$Q_{\text{back}}$</td>
<td>backscatter efficiency</td>
</tr>
<tr>
<td>$Q_{\text{ext}}$</td>
<td>extinction efficiency</td>
</tr>
<tr>
<td>$Q_{\text{sca}}$</td>
<td>scattering efficiency</td>
</tr>
<tr>
<td>$r$</td>
<td>particle radius</td>
</tr>
<tr>
<td>$s$</td>
<td>most probable size parameter</td>
</tr>
<tr>
<td>$T$</td>
<td>transmission</td>
</tr>
<tr>
<td>$R$</td>
<td>lidar ratio</td>
</tr>
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<td>$x$</td>
<td>particle size parameter</td>
</tr>
<tr>
<td>$x_m$</td>
<td>median size parameter</td>
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<tr>
<td>$x_{\text{rel}}$</td>
<td>relative particle size parameter</td>
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<td>$x_{\text{rms}}$</td>
<td>root-mean-square particle size parameter</td>
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<tr>
<td>$x_1$</td>
<td>core particle size parameter</td>
</tr>
<tr>
<td>$x_2$</td>
<td>coat particle size parameter</td>
</tr>
<tr>
<td>$x_i$</td>
<td>either core or coat particle size parameter</td>
</tr>
<tr>
<td>$\zeta$</td>
<td>mass extinction coefficient</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>empirical parameter in modified gamma size distribution</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>empirical parameter in modified gamma size distribution</td>
</tr>
<tr>
<td>$\theta$</td>
<td>scattering angle</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>wavelength of radiation in surrounding medium</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>$\lambda_{\text{rel}}$</td>
<td>relative wavelength of radiation in medium</td>
</tr>
<tr>
<td>$\lambda_{\text{vaco}}$</td>
<td>wavelength of radiation in vacuum</td>
</tr>
<tr>
<td>$\mu$</td>
<td>parameter used in gamma particle size distribution</td>
</tr>
<tr>
<td>$\xi$</td>
<td>aspect ratio</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>geometric deviation of log-normal size distribution</td>
</tr>
<tr>
<td>$\phi$</td>
<td>orientation angle</td>
</tr>
<tr>
<td>$\Omega$</td>
<td>solid angle</td>
</tr>
<tr>
<td>$\omega$</td>
<td>single scattering albedo</td>
</tr>
</tbody>
</table>
AN INTERACTIVE PROGRAM FOR ESTIMATING EXTINCTION AND SCATTERING PROPERTIES OF MOST PARTICULATE CLOUDS

1. INTRODUCTION

The interaction between electromagnetic radiation and suspended particulates is of great importance to many phenomena of scientific and military interest. These include atmospheric visibility, the propagation of laser beams through clouds and smokes, obscurants, laser or solar reflectance problems (e.g., lidar, IR proximity fuzes and thermal imaging) and multiple scattering. Also many common sights, such as blue sky, white clouds, glories and rainbows, can be explained by this interaction.

To date there is no general computer program available to calculate a wide variety of situations, despite the fact that there has been, for a number of years, a significant requirement. Part of the reason is that each particle shape poses problems unique to itself and thus a solution, for one shape only, requires a considerable investment of time. Also there is often only one specific end-use in mind.

To estimate, in general, how a particular wavelength of radiation will interact with a cloud of particles, the following are usually required: the shape of the particles, the optical constants of the material comprising the particles (i.e., the refractive index or dielectric constant), the particle size distribution throughout the cloud, the concentration and, for non-spherical shapes, the orientation distribution. Also the polarization state of the incident radiation may be required. Once this information is known or estimated and a suitable computer code is available, then the extinction and scattering properties of individual particles or a cloud of particles can be calculated.

This report is a description of a program to help meet most scattering problems for a variety of shapes and particle size distributions. Section 2 outlines the general considerations of the program followed by individual sections on the various particle shapes. These are: Section 3 Spheres and Coated Spheres; Section 4 Infinite Cylinders (including homogenous, coated and randomly oriented cases); Section 5 Finite Cylinders (oriented and random); and Section 6 Irregular Shapes (all random orientation). Additionally, Section 7 covers polydispersions, so that size distribution effects can be considered. Three appendices have also been included: Appendix A to illustrate some actual interactive cases, Appendix B to detail significant errors that were uncovered in the various texts and papers used and
Appendix C a listing of the FORTRAN 77 files and how to modify the program.

It is not intended that this report detail the physics that underlies the program since ample references will be given to readily obtainable material. It is recommended that the reader, wishing to familiarize himself with the concepts, application etc. of this program, read part or all of the following excellent texts: Van de Hulst (1957), Kerker (1969) and/or Bohren and Huffman (1983). Ruck et al (1970) and Bowman et al. (1987) can be used as supplementary texts.

2. GENERAL CONSIDERATIONS

i. Accuracy

Emphasis has been placed on the accuracy and generality of the codes. Extensive comparisons with this code and available experimental data as well as with independent calculations have been made with a high degree of success. For example, all the relevant diagrams in the texts mentioned at the end of the Introduction have been reproduced without error. Furthermore all the papers containing tables or diagrams of the scattering quantities of interest, in journals such as Applied Optics, have been verified. All the codes have been checked in the small (Rayleigh) and large (geometric optics) particle size limits where particularly simple theoretical expressions are well known. In particular the backscatter coefficient, one of the most sensitive indicators of the accuracy of a scattering code, must equal, in the limit of large particle size and absorption, the Fresnel reflection coefficient -independent of shape. All codes have passed these tests. There are however still other sets of parameters for which no experimental results or independent calculations exist and for which simple theoretical formulae do not exist. The only possible check in this case is that the program has internal agreement. This means reducing one particular shape calculation, by suitable choice of parameters, to another shape that exists in the code. For example, coated sphere to sphere, or coated infinite cylinder to infinite cylinder or finite cylinder to infinite cylinder. Excellent agreement, within theoretical limitations, is always found.

ii Approximate Timing

In this sub-section the approximate computing time that is required for the various codes for different particle sizes is given. The times are shown in Table 1 and are for runs on the VAX 8700. Two cases, with and without the phase function, are displayed. The efficiencies, mass extinction coefficient and the lidar ratio (all defined in section iii below) are always computed. It is not claimed that the program and the various subroutines are the most efficient. However most execution times that have been encountered are deemed to be reasonable. Long execution times, occurring for very demanding situations, such as polydispersions of large randomly oriented non-spherical particles, can be performed in batch mode.
**TABLE 1**

Approximate CPU times, in seconds, for running the different randomly oriented monodispered particle shapes on the MRL 8700.

No phase function required

<table>
<thead>
<tr>
<th>Size</th>
<th>Sphere</th>
<th>Coated Sphere</th>
<th>Coated Infinite Cylinder</th>
<th>Coated Infinite Cylinder</th>
<th>Finite Cylinder</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.1</td>
<td>0.1</td>
<td>2.9</td>
<td>4.2</td>
<td>0.1</td>
</tr>
<tr>
<td>10</td>
<td>0.1</td>
<td>0.1</td>
<td>5.7</td>
<td>8.5</td>
<td>0.15</td>
</tr>
<tr>
<td>20</td>
<td>0.1</td>
<td>0.1</td>
<td>8.2</td>
<td>11.7</td>
<td>0.16</td>
</tr>
<tr>
<td>40</td>
<td>0.13</td>
<td>0.11</td>
<td>12.6</td>
<td>18.2</td>
<td>0.18</td>
</tr>
<tr>
<td>75</td>
<td>0.15</td>
<td>0.13</td>
<td>20.3</td>
<td>29.8</td>
<td>0.27</td>
</tr>
<tr>
<td>100</td>
<td>0.16</td>
<td>0.15</td>
<td>25.4</td>
<td>37.4</td>
<td>0.31</td>
</tr>
<tr>
<td>200</td>
<td>0.19</td>
<td>0.17</td>
<td>46.1</td>
<td>66.8</td>
<td>0.55</td>
</tr>
<tr>
<td>500</td>
<td>0.36</td>
<td>0.26</td>
<td>106.0</td>
<td>185.9</td>
<td>1.21</td>
</tr>
<tr>
<td>750</td>
<td>0.49</td>
<td>0.36</td>
<td>159.7</td>
<td>235.6</td>
<td>1.72</td>
</tr>
<tr>
<td>1000</td>
<td>0.62</td>
<td>0.45</td>
<td>-</td>
<td>-</td>
<td>2.20</td>
</tr>
</tbody>
</table>

Phase Function at 10° intervals

<table>
<thead>
<tr>
<th>Size</th>
<th>Sphere</th>
<th>Coated Sphere</th>
<th>Coated Infinite Cylinder</th>
<th>Coated Infinite Cylinder</th>
<th>Finite Cylinder</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.13</td>
<td>0.13</td>
<td>6.0</td>
<td>7.1</td>
<td>1.71</td>
</tr>
<tr>
<td>10</td>
<td>0.13</td>
<td>0.13</td>
<td>12.0</td>
<td>14.2</td>
<td>9.0</td>
</tr>
<tr>
<td>20</td>
<td>0.13</td>
<td>0.13</td>
<td>17.5</td>
<td>20.7</td>
<td>25.2</td>
</tr>
<tr>
<td>40</td>
<td>0.16</td>
<td>0.14</td>
<td>27.3</td>
<td>33.2</td>
<td>-</td>
</tr>
<tr>
<td>75</td>
<td>0.20</td>
<td>0.16</td>
<td>44.4</td>
<td>53.5</td>
<td>-</td>
</tr>
<tr>
<td>100</td>
<td>0.24</td>
<td>0.20</td>
<td>54.3</td>
<td>66.7</td>
<td>-</td>
</tr>
<tr>
<td>200</td>
<td>0.38</td>
<td>0.32</td>
<td>101</td>
<td>124</td>
<td>-</td>
</tr>
<tr>
<td>500</td>
<td>0.81</td>
<td>0.64</td>
<td>231</td>
<td>300</td>
<td>-</td>
</tr>
<tr>
<td>750</td>
<td>1.14</td>
<td>0.88</td>
<td>347</td>
<td>437</td>
<td>-</td>
</tr>
<tr>
<td>1000</td>
<td>1.43</td>
<td>1.12</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
In the table, two cases are considered. Firstly, where no phase function is required, and, secondly, where the phase function is required at intervals of $10^\circ$. For non-spherical particles random orientation is used. In all cases the particles are monodispersed. From this table it is possible to estimate the amount of computer time a given case will take and thus if it is reasonable.

The program also runs on the MRL VAX 780. The computation times in this case are about 3-5 times longer than those listed in Table 1.

iii Using the Program

The main program IPHASE and its subroutines have been created on the MRL VAX 8700 in standard FORTRAN 77. Very little, if any, sophisticated programming was required so that the entire program should be readily transportable. Before using the program, unit number 7 should be properly set. This will determine where the numerical output will go. This can be done on a VAX by ASSIGN MYFILE FOR007 to have the data go to MYFILE or by ASSIGN SYS$OUTPUT FOR007 to have the data go to the terminal screen. All other information will appear on the terminal screen. In order to run the program, RUN IPHASE, must be entered on a suitable terminal. From then on the program will prompt the user for the required information such as particle shape, refractive index, particle size parameter etc. All information, except where noted, should be nondimensional. The individual sections describing each particle shape detail exactly what information will be required. On output the program will give the phase function over the angles requested, the extinction, scattering and absorption efficiencies, the mass extinction coefficient and, if the backscattered part of the phase function was asked for, the lidar ratio.

The following gives a very brief description of the above items.

The phase function, $p(\theta)$, gives the relative probability of the incident light to be scattered at an angle $\theta$ from the incident direction. It is normalized to 1 over the solid angle, i.e.

$$\int_0^{2\pi} p(\theta) d\Omega = 1,$$  \hspace{1cm} (1)

It governs the way in which the light will propagate through the cloud and is essential, for example, in the study of cloud reflectance and multiple scattering.

The extinction, scattering and absorption efficiencies, $Q_{ext}$, $Q_{sca}$, and $Q_{abs}$ respectively, indicate how well the particle or distribution of particles cause extinction, scattering and absorption of the incident light. They are defined as the appropriate cross section per unit projected area. Thus if $C_{ext}$ is the extinction cross section, and $\Delta$ the projected area, then

$$Q_{ext} = \frac{C_{ext}}{A}.$$  \hspace{1cm} (2)
Note that for a sphere \( A = \pi r^2 = \lambda^2 x^2 / 4 \pi \) where \( r \) is the particle radius, \( x = 2 \pi r / \lambda \) is the size parameter, and \( \lambda \) is the wavelength. The other efficiencies are similarly defined. The larger the value of the extinction efficiency the better the particle is at attenuating the beam in the incident direction.

The mass extinction coefficient, \( \alpha \), is closely related to the extinction efficiency and cross section by

\[
\alpha = \frac{A Q_{\text{ext}}}{M} = \frac{C_{\text{ext}}}{M}
\]

(3)

where \( M \) is the mass of the particle. This indicates how effectively, per unit mass, a particle or system of particles attenuates a beam of light. This number is of central interest to the obscuration sciences and determines the transmission through a given cloud or smoke. Thus, if \( I_0 \) is the incident intensity of the incoming radiation, \( C \) is the concentration of aerosol and \( I \) is the intensity of the radiation after travelling a distance \( L \) through the cloud then the transmission is defined by

\[
T = \frac{I}{I_0} = e^{-\alpha CL}.
\]

(4)

The lidar ratio, proportional to the ratio of backscatter to extinction, allows for the calculation of the extinction from the backscatter (as in lidar) or the backscatter from the extinction. It is defined by

\[
R = \frac{1}{4\pi} \frac{Q_{\text{back}}}{Q_{\text{ext}}} = p(180^\circ) \frac{Q_{\text{scat}}}{Q_{\text{ext}}}
\]

(5)

where \( Q_{\text{back}} \) is the backscatter efficiency. Thus estimates of the particle concentration can be obtained if the lidar ratio, backscatter and mass extinction coefficient are known.

The complex refractive index, \( m = n - ki \), is the refractive index of the material relative to the surrounding medium. Here \( n \) is the real part (scattering) and \( k \) is the imaginary part (absorption) of the refractive index. Therefore the refractive index to be input into the program is the refractive index of the bulk material divided by the refractive index of the medium. Usually the medium is air which has \( m = 1 - 0i \) to a good approximation and thus, for this case, there is no difference between the two material refractive indices. Care must also be taken with the size parameter. As the definition of \( x \) involves \( \lambda \) and \( \lambda \) changes as the refractive index changes \( x \) must be changed accordingly. So \( x_{\text{rel}} = nx \) and \( \lambda_{\text{rel}} = \lambda_{\text{vac}} / n \) where \( \lambda_{\text{vac}} \) is the wavelength in a vacuum. For example, if the problem is the scattering of bubbles in water then \( m_{\text{rel}} = (1 - 0i) / (1.33 - 0i) = 0.75 - 0i \) where \( m_{\text{rel}} \)
is the relative index of refraction of the bubble to water (with bulk index $1.33-0i$). Also $x_{\text{rel}} = 1.33x$ and $\lambda_{\text{rel}} = \lambda_{\text{water}}/1.33$.

Some of the above quantities are sensitive to the polarization state of the incident radiation. The incident radiation can have several different states of polarization. These are linear, circular, elliptical and random. Since both circular and elliptical can be readily computed from the linear polarization states, only linear and random states need be considered. Linear polarization is typical of laser radiation while random polarization is commonly the form of white natural lighting. Radiation from a laser can be linearly polarized parallel or perpendicular to the scattering plane, which is the plane containing the incident radiation and the scattered radiation. So, in order to give a complete description of scattering, the program will prompt the user, when necessary, for the desired polarization state, the choices being polarization states parallel, perpendicular or random with respect to the scattering plane. These choices are presented to the user for two cases: 1. when the particle shape is spherical and some part of the phase function is required and 2. randomly oriented infinite cylinders. All other cases, such as oriented infinite cylinders or finite cylinders, assume random polarizations in order to simplify what would otherwise be a more complicated situation. Again, excellent discussions of polarization can be found in any of the scattering texts mentioned in the introduction.

iv Limitations

Any computer program has some form of limitations. This scattering code is no exception. Although a good deal of effort has been spent to restrict the limitations of each sub-program there are many that remain. The limitations are found to be caused by one of three reasons: memory, numerical and theoretical.

Table 2 summarizes for all the codes the various limitations found in each of the different particle shapes. The limitations are imposed on the size, in terms of $z$, refractive index, $m$ and a function of both $m$ and $x$. In addition there is some limitation on the choices of coating sizes in the case of coated particles. The limitations listed in Table 2 give a basic idea of the expected range of validity. However, combinations of some of the extreme values of these parameters may also cause problems.

The memory limitations are imposed by the fixed array sizes that are required by FORTRAN 77 or by the finite size of memory that is allocated to a user’s workspace. As the array sizes actually used are large, only in extreme cases should this type of limitation be of concern. Memory limitations is the reason for the limit in size that is listed in Table 2 for all shapes except the finite cylinder and irregular particles. For the latter shapes other limitations appear well before the memory limitations. An example of a memory limitation is using a size parameter $z$ of 3000 in the sphere routine.

The numerical limitations are much more of a problem and generally result from the finite precision of the word structure in FORTRAN 77. Numerical problems caused by overflow or underflow are obvious and will be indicated by the computer itself. Usually these occur when intermediate values of Bessel functions or Hankel functions are very large. An example of this kind of limitation would be a calculation involving spheres with
TABLE 2

Limitations to the various particle shapes as expressed in terms of the size parameter $x$, the refractive index $m$ and both $m$ and $x \cdot \phi$ is the orientation angle and the subscripts $1,2,i$ refer to the core, coating or either respectively.

<table>
<thead>
<tr>
<th>Shape</th>
<th>Size</th>
<th>$m$ and $x$</th>
<th>$m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sphere</td>
<td>$6 \times 10^{-5} \leq x \leq 2300$</td>
<td>$</td>
<td>m</td>
</tr>
<tr>
<td>Coated Sphere</td>
<td>$5 \times 10^{-7} \leq x_2 \leq 1050$</td>
<td>$\text{Im}(m_1 x_1), \text{Im}(m_2 x_1), \text{Im}(m_2 x_2) \leq 30$; \text{Im}(m_2 x_2) \leq 30$; \text{Re}(m_i) \leq 1, then $x_2 \leq 200 \text{Re}(m_i)$</td>
<td>$</td>
</tr>
<tr>
<td>Infinite Cylinder</td>
<td>$3 \times 10^{-5} \leq x \sin \phi \leq 950$</td>
<td>$</td>
<td>x(m^2 - \sin \phi)^\frac{1}{2}</td>
</tr>
<tr>
<td>Coated Infinite Cylinder</td>
<td>$1.7 \times 10^{-6} \leq x \sin \phi \leq 950$; $10^{-19} \leq \frac{x_1}{x_2} &lt; 1$</td>
<td>$\text{Im}(m_2 x_2) \leq 30$; $\text{Re}(m_i) &lt; 1, x \leq 660 \text{Re}(m_i) + 15$</td>
<td>$3 \times 10^{-3} \leq</td>
</tr>
<tr>
<td>Oriented Finite Cylinder</td>
<td>$10^{-12} \leq L \sin \phi \leq 10^{37}$</td>
<td>None</td>
<td>$0 \leq</td>
</tr>
<tr>
<td>Random Finite Cylinder</td>
<td>$.75 \leq L \leq 20$; $10^{-7} \leq x \leq .5$; $O's$ only; $L &gt; 20$ and $L &gt; 5$</td>
<td>None</td>
<td>As Oriented Finite Cylinder</td>
</tr>
<tr>
<td>Irregular</td>
<td>$.1 \leq x \leq 50$</td>
<td>$</td>
<td>m</td>
</tr>
</tbody>
</table>
\[ x = 10^{-7} \] which causes overflow. More serious still are numerical instabilities which may give reasonable-looking results but are nevertheless incorrect. The program is designed to anticipate most of the common numerical instabilities where they were impossible to eliminate entirely. In cases of extreme or unusual input parameters extra care with the results is suggested. An example of this situation is in the case of the coated sphere with core and coat refractive indices \( m_1 = m_2 = 0.5 - 0i \) and \( x = 20 \).

Theoretical limitations occur, except in trivial circumstances, with the particle shapes that do not have exact solutions. The reason for a given limitation can be traced to the approximations required to bring about a solution. Thus, for example, the variational solution for finite cylinders assumes that the cylinder is much longer than the width. If the length to diameter ratio is significantly less than 10, erroneous results will most likely result. See section 5 for further details. Another example is the code for irregular particles which assumes that the semi-empirical parameters employed are always valid. It is highly unlikely that these parameters are universal implying a varying degree of error in the results.

3. SPHERES AND COATED SPHERES

i Homogeneous Spheres

The general solution to scattering from spheres was first derived in 1890 by Lorentz and by Mie (1908) and now forms the classic method of solving scattering problems from particles. In outline, the wave equation is derived from Maxwell's equations assuming spherical spatial coordinates. By separation of variables and imposing boundary conditions on the electromagnetic fields, the phase function and related scattering properties of the sphere can be obtained. This solution is in terms of 'Mie coefficients' which are in turn represented by half-integer order Bessel functions of the first and second kind and their derivatives. Thus the solution to the homogeneous sphere is reduced to the calculation of the half-integer order Bessel functions. The full details are in any of the three texts mentioned in the introduction.

The Bessel functions have been calculated according to the known recipes and caveats (see Abramowitz and Stegun 1964 or Bohren and Huffman 1983). Thus backward recurrence is used when forward recurrence is unstable making the Bessel functions quite reliable.

The sphere code, MIEPHASE, is written in double precision since this case is used extensively and there are many interesting resonances that require the added accuracy. The input requirements are only the refractive index and particle size distribution and, if the phase function is requested, the polarization state of the incident radiation.

Applications for the sphere code are numerous. A few examples are naturally occurring water clouds, fogs, liquid pollution aerosols, bubbles in water, phosphorus or oil smokes and colloidal suspensions.
ii Coated Sphere

The coated sphere solution was first derived by Aden and Kerker (1951). The method of solution is very similar to that of the homogeneous sphere, albeit more complicated. Again half-integer order Bessel functions and their derivatives are used.

The program employed, COAT, is substantially copied from the listing in the Appendix of Bohren and Huffman (1983). Modifications have been made to make the code more reliable and to produce the phase function. The stated limitations on $mr$ and listed in Table 2 remain however. It seems impossible to obtain some of the required Bessel functions for large, absorbing spheres because of the exceedingly large numbers involved in the intermediate calculation.

The code is in single precision and thus runs $10-20\%$ faster than the double precision homogenous code. The input requirements are the refractive index of the core and coating, the size of the core relative to the coating and the particle size distribution. In the case of polydispersions the user has the choice of keeping the core size constant or the ratio of core size to coating size constant. Also, as with the homogeneous case, the polarization state of the incoming radiation is required if any part of the phase function is desired.

Some applications of the coated sphere are bubbles in the air, foam, water coated hail and oil coated metallic particles.

4. INFINITE CYLINDERS AND COATED INFINITE CYLINDERS

i Homogeneous Infinite Cylinders

The solution for infinite cylinders of arbitrary orientation and refractive index was first obtained in Wait (1955). Note that here infinite can mean, to a good approximation, that the length of the cylinder is much greater than the wavelength considered. It is found that a cylinder can be considered 'infinite' if $L > 200$, where $L$ is the length size parameter of the cylinder i.e. $L \equiv 2\pi l/\lambda$ where $l$ is the length of the cylinder. The procedure is the same as for spheres except cylindrical coordinates are used. The resulting solution is in terms of the integer order Bessel functions of the first and second kind. The prescription for the calculation of the phase function and the other output quantities follows that of Kerker (1969).

The single precision code, CYLINDERPHASE, requires as input the refractive index, the size parameter or size distribution of the radius and the orientation. The polarization state of the incident radiation is required for random orientations only. Unpolarized radiation is assumed for fixed orientations. Unlike spheres, all other shapes in general scatter quite differently if the orientation is changed. The orientation of an infinite cylinder is usually described by the angle the incident radiation makes with the cylinder axis. Thus perpendicular incidence means that the orientation is at $90^\circ$, the other angles being simi-
larly defined. It is to be noted that if the phase function for an oriented infinite cylinder is required then the output will be the phase function around the cone of scattering. This is because the infinite cylinder does not scatter in any other direction. This will be indicated by the program for this case. Details of the scattering geometry are best described in Kerker (1969) p263-4.

Normally, an orientation angle of 0° for an infinite cylinder would give no extinction or scattering. Since this case does not provide any useful information, entering a value of 0 for orientation angle in the program will produce instead results for random orientation. Random orientation is the case which will be the most frequently encountered. However, there are important conditions when clouds of cylinders may be oriented or partially oriented which commonly occurs with falling ice crystals. The case of randomly oriented infinite cylinders is interesting since the first published case of a successful calculation, free of singularities, was as late as 1985 (Haracz et al 1985). Previous solutions must attempt to remove singularities that occur in the computation (Mckay and Timusk 1984 and Stephens 1980) or may predict no backscatter (Liou 1972). The difficulty, surprising at first, occurs because the scattered radiation occurs along the surface of a cone which is infinitely thin. Thus just numerically integrating over all possible orientations will not work since this must be a finite integration. However by a suitable coordinate transformation and properly weighting the integration a satisfactory algorithm can be written.

It should be noted that the computation times for randomly oriented infinite cylinders are considerably longer for a particular radius than those for the sphere of similar size. This occurs since all the possible orientations must be considered involving two independent angles.

The infinite cylinder scattering program can be applied to long fibres (as in insulation material, asbestos fibres, chaff at small wavelengths), spider webs and even some viruses. The main use to date is the scattering of micro- and radio waves from long antennas and other objects.

ii Coated Infinite Cylinders

The most general case for coated infinite cylinders would require that both the refractive index of the core and coat and also the orientation be arbitrary. No solution to this problem has yet been derived. The most general case that has been solved is for arbitrary orientation and arbitrary coating but a perfectly conducting core. As this is usually well approximated by a coated metal this is still useful.

The coated conducting infinite cylinder for oblique orientation was first obtained by Tang (1957). The solution used here was given by Thomas in 1963 and can be found in Ruck (1970). The representation is in terms of surface impedances and surface admittances but still requires the integer Bessel functions as does the homogeneous case. Thus, as in the case of spheres, the coated particle calculation is similar but more complicated than the homogeneous case.

This single precision code, COATCYL, requires the refractive index of the coat, the
relative size of the core to coat and the orientation of the particles. Polarization considerations are as for the homogeneous case above. Again a choice is available for holding the core radius constant or the ratio of core to coat radii constant as was done for the coated sphere. Similar to the homogeneous case an orientation of 0° means random orientation. This routine can be used for calculating scattering parameters of infinite cylinders with infinite refractive index (i.e., perfect conductors). This is done by setting the coating refractive index to 1 - 0i and the ratio of the core to coat radius to 0.9999999.

This algorithm has been applied to incoming meteors and re-entry problems as well as scattering of microwave and radar radiation.

5. FINITE CYLINDERS

Scattering by finite cylinders has been studied intensively since World War II and with the invention of radar for the purpose of scattering from antennas. No exact solution has yet been obtained since a finite cylinder has ends and thus edges. Edges always cause serious problems in the theory of scattering. The best solutions that exist assume that the length of the cylinder is much larger than the radius (and thus the edge effects can be ignored). Thus, the antenna approximation implies that the radiation induced current in the wire is confined to the centre of the wire. Usually L/x ≥ 10. Also implied is that this current is zero at the ends of the wire. The variational approach is used in this code. The code follows that found in Pederson et al (1984, 1985). Other approximations exist (e.g., the direct method Bowman et al 1987) but they are only for perfectly conducting materials. These are the only references that give a procedure for calculating the scattering information of obliquely oriented finite fibres of arbitrary refractive index (although the central equations were written by Van Vleck et al 1947 and Tai 1951). Random orientations are also included (Waterman et al 1984). Unlike the previous exact solutions the starting point is to match the surface currents (produced by the incident radiation and induced current in the wire) upon the finite cylinder or wire. This is simply a statement of the conservation of energy. The variational method is then employed, as is standard in many problems in physics, to obtain the solution. All of the above references should be consulted if more detail of the algorithm is required. The variational technique for solving differential equations is detailed, for example, in Bowman (1987).

The solution, although complicated, requires the evaluation of sines and cosines and the sine and cosine integrals all of which are relatively straightforward. The main complication is the evaluation of the surface impedance for finite conductivities. This is further complicated if the radius of the cylinder is sufficiently small so that electron scattering from the sides of the cylinder must be considered. In the latter case, the program, if so required, will ask for the appropriate information as needed in order to make the corrections to the bulk refractive index. For details of the physics of this adjustment see Kittel (1968).

The oriented code, FIBER, has, in addition to the variational method, various approximations to extend its range of validity. The randomly oriented code, RANDOMF, uses
only the variational method as mentioned above. In order to detail this better first define the length size parameter as \( L = 2\pi l/\lambda \) and the radius size parameter as \( x = 2\pi r/\lambda \) where \( l \) is the length and \( r \) is the radius of the finite cylinder or fibre. Also let \( \xi = L/2x \) be the aspect ratio. Then for the variational code to be considered accurate \( 0.75 \leq L \leq 20, \quad x \leq 0.5 \) and \( \xi > 5 \). If \( L \leq 4 \) and \( x \leq 0.4 \) the Rayleigh, or small particle approximation is employed. If neither of these two conditions is satisfied but \( L > 5, x \leq 10 \) and \( \xi > 1.5 \) then a long cylinder approximation due to Van de Hulst (1957) is used. Finally, if the case is still different then there are no suitable approximations and the calculation is aborted. These various approximations have not been included into the code for random orientation because at the boundaries of the above conditions the calculation for one approximation will differ from the other thus creating nonphysical jumps in the calculated quantities as the boundaries were crossed. Additionally these would be averaged out in randomization giving an answer with unknown errors. The approximations have been provided to allow the user to explore finite cylinder scattering beyond the limits of the variational approximation and to delineate the potential errors in the random code. As shown in Table 2 the limitation of \( L \leq 20 \) can be lifted if the phase function is not required. Thus the accuracy of the efficiencies seem to extend well beyond the range of the approximation. See Pederson et al. (1984) for more details.

This single precision code requires as input the refractive index, the radius size parameter, length size parameter and the orientation angle. The incident polarization state is always assumed to be random i.e. unpolarized. As for infinite cylinders, \( 0^\circ \) implies random orientation. Additionally, if the radius of the particle is very small (i.e. \( \leq 0.6 \mu m \)) then further information is required in order to calculate the effect of this small size, as alluded to above, on the refractive index. The additional information is: the bulk conductivity, specific gravity, molecular weight and the number of conduction electrons per molecule. All units of the previous quantities must be expressed in SI units. The calculation will not be able to make the required adjustment in the refractive index if the fibre radius is too small (about 100-200 Å).

Since the scattering from a finite cylinder varies over the two angular directions, the phase function is given, for oriented fibres, only in the scattering plane (the plane containing the incident radiation and the cylinder axis). A slight modification of the code would allow for the scattering in other planes. For random orientations the meaning of the phase function is the same as for spheres and randomly oriented infinite cylinders.

This code is important for studies concerning chaff to block radar or microwaves and 'mini-chaff' or coatings for blocking millimetre waves.

6. IRREGULAR SHAPES

As no exact code exists for the general irregular particle shapes different approaches are required. A great variety of techniques have been used with varying degrees of success and to write individual codes for each would be very time consuming and of questionable
value. However there is a semi-empirical approach that can be used for randomly oriented irregular shapes for $x = 0$ to $\approx 50$. This is the approach given by Pollack and Cuzzi (1979).

This algorithm assumes that for particles with size parameters $\leq 5$ the Mie theory for spheres can be used. The exact size depends on the chosen shape. This has been verified to be a reasonable approximation for many different shapes. For the larger particles the contribution to the scattering is broken down into three parts: diffraction, external reflection and transmission.

The diffraction component is calculated by use of physical optics. Assuming convex particles this contribution is proportional to a first order Bessel function.

The external reflection is calculated by consideration of geometrical optics. Thus the reflection is easily computed in terms of the Fresnel reflection coefficients.

The transmission is simply modelled by an exponential that is properly normalized. It is considered that a more exact treatment would be too difficult if not impossible to achieve.

This semi-empirical approach has been compared to many experimental data with satisfactory results. It is noted however that extra caution is required if the particle type is highly absorbing and elongated. For these cases the finite cylinder model may be preferred.

The 'shape' is defined by 3 numbers that define the ratio of surface area to the surface area of an equal volume sphere, the degree of sphericity, and the degree of surface roughness. For the degree of sphericity, 1 would be used for particles that are sphere-like and 5 should be used for particles that are flake-like. Numbers in between can be used to specify the varying degrees of sphericity. Likewise the roughness is defined by a number between 1 and 10. Very rough particles are indicated by 1 and smooth particles are represented by 10.

The code is written in single precision and requires the refractive index and the size distribution (which cannot be monodispered). Unpolarized incident radiation is assumed. The output gives the phase function and the various contributions to it. The phase function for the small spheres is given, with the phase functions for the diffraction, reflection and transmission components. Also given is a similar breakdown of the efficiencies, the fraction $F$ of the particles in the larger, non-Mie, size regime and the root-mean-square particle size $x_{rms}$.

This code can be used to indicate how irregular particles will change the extinction and phase function from that of regular particles and where the major contributions come from. It has been used for explaining why and by how much particle irregularity will affect resonances that are observed in regular shapes.
7. POLYDISPERSIONS

In most real situations, the particles constituting the cloud will be polydispersed or occur in different sizes. These size distributions can be in many different forms and can affect significantly the scattering behaviour of a cloud. For this situation, the calculation of the scattering properties must be performed over all the sizes occurring in the cloud with the desired size distribution used as the weighting function. The program will ask for the desired integration step and integration limits. Small enough integration steps should be used in order that proper convergence is obtained. As is typical for numerical integration, several values of the integration step size may be needed to indicate if convergence to the correct values has occurred. The integration limits over the particle size parameter can vary anywhere between 0 and 500. If, from the construction of the size distribution, there are one or more narrow peaks, care is needed to ensure that the integration step size is small enough to include the peak properly. To easily verify this the user can, if desired, display the size distribution in tabular form.

Five different particle size distributions, other than monodisperse, have been included in the program. In addition to this, the user can compose a multi-modal distribution made up of any number of the different distributions offered. This option allows for studying the effects, often encountered, of different populations of particles in the cloud.

The five polydispersions that can be chosen are described as follows:

- The Gates-Gaudin-Schumann size distribution, usually used for fine aerosols naturally occurring in the atmosphere, is defined simply as

\[ F(x) \propto x^{-a} \]  

where \( a \), the only parameter, is typically about 2 or 3. Note that this distribution becomes infinite as \( x \to 0 \). Thus there must be some non-zero cutoff applied to the distribution.

- The log-normal distribution is used frequently in modelling aerosols, especially natural water clouds and other liquid particulate clouds. It is defined by

\[ F(x) \propto \frac{1}{\sigma x} e^{-\frac{(\ln x - \ln x_m)^2}{2\sigma^2}} \]  

where \( \sigma \) is the geometric deviation of the distribution and \( x_m \) is the median size. Thus \( x_m \) gives the average size of the particles and \( \sigma \) the width of the distribution. Typical values for \( \sigma \) are between .1 and 2.
A third choice of size distribution is the gamma distribution. Like the log-normal distribution it is often used in natural water clouds and fogs. The choice of this or the log-normal distribution depends on goodness of fit to an experimental distribution or perhaps some advantageous mathematical property. The gamma distribution is defined as

\[ F(x) \propto \frac{1}{\Gamma(\mu + 1)} \mu^{\mu+1} x^{\mu} e^{-x/\mu} \]  

where \( s \) is the most probable size and the half-width of the distribution can be characterized by \( \frac{1}{\mu+1} \). Typical values for \( \mu \) range from 2 - 10.

A distribution that has been used in many calculations, and a standard set of aerosol models is based on it, is the modified gamma distribution. It is defined as

\[ F(x) \propto x^\alpha e^{-bx^\gamma} \]  

Here \( b, \alpha, \gamma \) are empirical parameters. Deirmendjian (1969) has defined many models by using the modified gamma distribution such as haze, rain and several cloud types. These are now widely used for the intercomparision of theoretical results.

A final distribution available in this program is the Rosin-Rammler distribution. It is one not often encountered in aerosols because it is intended for use as a model size distribution of powders (such as coal) and cases where the particles were formed by crushing and sieving. It is very useful in describing many solid particulate distributions. It is defined as

\[ F(x) \propto x^{n-1} e^{-bx^n} \]  

where \( b \) is a measure of width of the distribution and \( n \) depends on the substance.

As previously mentioned some situations call for distributions with two or more peaks. These cannot be easily modeled by a single analytic function. Instead they are modeled by a sum of simpler functions. This scattering program allows for the sum of any number of the above distributions. As each is entered to form the multi-modal distribution the program will prompt the user to indicate the relative importance that each distribution has so that a weighted sum can be formed.

It is to be noted that in the above distributions, (6)-(10), there is no need to indicate the particle number or concentration and hence all multiplicative constants have been dropped. Therefore these distributions themselves are not normalized. This is because the calculations are all performed, where possible, non-dimensionally. Thus, after the calculation is executed, the particle concentration can be considered and changed without recalculation.
8. CONCLUSIONS

An interactive program has been written to meet most radiative propagation needs in particulate suspensions. The program can calculate the phase function, the extinction, scattering and absorption efficiencies, the mass extinction coefficient and lidar ratio for the following particle shapes: homogeneous spheres, coated spheres, homogeneous infinite cylinders, coated infinite cylinders, finite cylinders and some irregular shapes. For all shapes, except the irregular shapes, the user has the choice between mono-dispersed or polydispersed particles. The irregular shapes must be polydispersed. The particle size distribution can be chosen from any of the five most commonly used distributions with the option of forming multi-modal distributions. A choice of oriented or random orientation is given for the non-spherical regular particles. Also, when appropriate, a choice of incident polarization states is allowed.

Timing information is supplied to allow for the estimate of the computation time for a given problem which is of use for demanding situations.

A comprehensive table listing the main limitations of the codes due to memory, numerical approximations or theory is discussed. The important theoretical limitations are further described in individual sections for each particle shape were appropriate.

Appendices are also given that give examples of the use of this program, briefly list the significant errors found in the literature and the modules used in creating the code.
9. REFERENCES


APPENDIX A

Some Representative Examples

In this appendix some examples will be given to illustrate how the program can be used to solve various scattering and related problems. In all the examples data the user must input is contained between the square brackets i.e. [1.33,0] means that 1.33, 0 is entered. Each line of input is to be terminated by hitting return on the terminal.

Example 1

The first example is simply to calculate the phase function at 10° intervals along with the efficiencies etc. of 5μm water particles. Unpolarized light at 0.55μm is assumed

$[ASS SYS$OUTPUT FOR007]
$[RUN I PHASE]
WHICH PARTICLE TYPE:
1) SPHERE EXACT
2) COATED SPHERE EXACT
3) INFINITE CYLINDER EXACT
4) FINITE CYLINDER 1ST ORDER VARIATIONAL
5) COATED INFINITE CYLINDER EXACT
6) CUBE SEMI-EMPIRICAL
7) OCTAHEDRA SEMI-EMPIRICAL
8) FLAKE SEMI-EMPIRICAL
9) CONVEX-CONCAVE SEMI-EMPIRICAL
10) OTHER IRREGULAR SEMI-EMPIRICAL

INDEX OF REFRACTION $m$ & $k$ ?
[1, 3.3, 0]
WHICH PARTICLE SIZE DISTRIBUTION (MODE= 1):
1) MONODISPERSED $X$
2) GATES-GAUDIN-SCHUMANN $X^{(-A)}$
3) LOG-NORMAL $1/(SG*X)*EXP(-(LOG(X)-LOG(XM))**2/(2*SG**2))$
4) GAMMA $U**(U+1)/(U+1)! *(R**U/S**(U+1))*EXP(-U*R/S)$
5) MODIFIED GAMMA $R**A*EXP(-B*R**G)$
6) ROSIN-RAMMLER $X**(N-1)*EXP(-B*X**N)$
7) MULTI-MODAL

DO YOU WANT ANY PART OF THE PHASE FUNCTION (YES=0) ?
[0]
ENTER LOWEST, HIGHEST AND INCREMENT OF ANGLES IN PHASE FUNCTION
[0, 180, 10]
WHICH POLARIZATION STATE? 1) PARALLEL
2) PERPENDICULAR
OR 3) RANDOM
WITH RESPECT TO SCATTERING PLANE.

ENTER PARTICLE SIZE OR LENGTH PARAMETER
[57.12]

Note that before the program is run, unit 7 is defined so that the output will go to the
terminal screen. Once defined this command need only be used again if the output is to
be sent somewhere else.

Now the program is executed. The first response of the program is to list the choices
of particle shape and then waits for the response. In this case the sphere Mie routine
is chosen. Next the program asks for the index of refraction which for water at 0.55μm
which is 1.33 - j0. The possibilities of the size distribution are next listed. Since, in this
example, only one size of particle is involved the monodispersed distribution is chosen. The
program now asks the user if any part of the phase function is required. The value 0 for
yes is entered in this case. Now the user must define which parts of the phase function are
required. As the phase function is usually defined between 0 - 180° we have entered here
0, 180, 10. This indicates that the phase function will be calculated from 0° to 180° every
10° as demanded by the example. Next the polarization state of the incident light must
be input. The random state was chosen as the incident light is assumed to be unpolarized.
The final question is the size parameter of the particles. Since the size parameter \( z = 2\pi r \lambda \)
we calculate from the numbers in the example that \( z = 57.12 \). The program then sends all
the output to the terminal screen. The output for this example was the following:

<table>
<thead>
<tr>
<th>Angle (°)</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>141.46</td>
</tr>
<tr>
<td>10.00</td>
<td>0.64879</td>
</tr>
<tr>
<td>20.00</td>
<td>0.39525</td>
</tr>
<tr>
<td>30.00</td>
<td>0.18270</td>
</tr>
<tr>
<td>40.00</td>
<td>0.51272E-01</td>
</tr>
<tr>
<td>50.00</td>
<td>0.23661E-01</td>
</tr>
<tr>
<td>60.00</td>
<td>0.12857E-01</td>
</tr>
<tr>
<td>70.00</td>
<td>0.93166E-02</td>
</tr>
<tr>
<td>80.00</td>
<td>0.47997E-02</td>
</tr>
<tr>
<td>90.00</td>
<td>0.22146E-02</td>
</tr>
<tr>
<td>100.00</td>
<td>0.37373E-02</td>
</tr>
<tr>
<td>110.00</td>
<td>0.22730E-02</td>
</tr>
<tr>
<td>120.00</td>
<td>0.25434E-02</td>
</tr>
<tr>
<td>130.00</td>
<td>0.11005E-01</td>
</tr>
<tr>
<td>140.00</td>
<td>0.40741E-01</td>
</tr>
<tr>
<td>150.00</td>
<td>0.10366E-01</td>
</tr>
<tr>
<td>160.00</td>
<td>0.58200E-02</td>
</tr>
<tr>
<td>170.00</td>
<td>0.26868E-01</td>
</tr>
<tr>
<td>180.00</td>
<td>0.71797E-01</td>
</tr>
</tbody>
</table>

QEXT = 2.1532931  QSCA = 2.1532931  QABS = 0.000000000E+00
MASS EXTINCTION COEF. = 0.17764626 / LAMBDA/DENSITY
LIDAR RATIO = 0.71796536E-01

The phase function is listed first. Each angle requested has the relative scattering probability beside it. After the phase function is $Q_{eff}, Q_{sca}$ and $Q_{abs}$. Since this particle is large with respect to the wavelength and there was no absorption (the 0 in the index of refraction) $Q_{eff} = Q_{sca} = 2$ and $Q_{abs} = 0$. Since the phase function was calculated at 180°, the lidar ratio was automatically calculated. Lastly, the mass extinction coefficient is presented. This quantity, unlike the others, has dimensions. Thus to get the mass extinction the number given must be divided by the density and the wavelength. For this case the density of water is 1 g/cm$^3 = 10^6$ g/m$^3 = 10^3$ kg/m$^3$ and the wavelength was $0.55 \mu m = 5.5 \times 10^{-4}$ m. Thus the mass extinction coefficient $\alpha = 0.5517764 / 5.5 = 1.003$ m$^2$ g$^{-1}$. 
In the next example, an atmospheric cloud containing 1% carbon and 99% aerosol by volume, produced by burning, is known to be monodispersed with 1μm particles. Assume that it is also known that at a critical distance from the cloud, a single scattering albedo greater than 85% will defeat a fuze operating at 1.06μm on an imaginary seeker. Which of the following two possibilities will defeat the fuze: when the carbon is uniformly mixed with the aerosol or when the carbon is contained as a nucleus in the aerosol particle? Assume that the refractive index of the carbon-water mixture is 1.55 – .007i, of carbon is 1.7 – .7i and of the aerosol is 1.55 – 0i.

Since the single scattering albedo ω = Q_{esc}/Q_{ext} the phase function is not required. However both the sphere and coated sphere models must be used. First the homogeneous sphere:

<table>
<thead>
<tr>
<th>WHICH PARTICLE TYPE</th>
<th>WHICH MONODISPERSED</th>
<th>WHICH GATES-GAUDIN-SCHUMANN</th>
<th>WHICH LOG-NORMAL</th>
<th>WHICH GAMMA</th>
<th>WHICH MODIFIED GAMMA</th>
<th>WHICH ROSIN-RAMMLER</th>
</tr>
</thead>
<tbody>
<tr>
<td>1) SPHERE EXACT</td>
<td>X</td>
<td>X**(-A)</td>
<td>1/(2 SG**2)</td>
<td>U**(-U+1)/(U+1)</td>
<td>R**(-B*R**G)</td>
<td>X**(-N-1)<em>EXP(-B</em>K**N)</td>
</tr>
<tr>
<td>2) COATED SPHERE EXACT</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3) INFINITE CYLINDER EXACT</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4) FINITE CYLINDER 1ST ORDER VARIATIONAL</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5) COATED INFINITE CYLINDER EXACT</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6) CUBE SEMI-EMPirical</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>7) OCTAHEDRA SEMI-EMPirical</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>8) FLAKE SEMI-EMPirical</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9) CONVEX-CONCAVE SEMI-EMPirical</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10) OTHER IRREGULAR SEMI-EMPirical</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

[1]

INDEX OF REFRACTION m & k?
[1.7, .007]

DO YOU WANT ANY PART OF THE PHASE FUNCTION (YES=0)?

[1]

ENTER PARTICLE SIZE OR LENGTH PARAMETER
[5.928]

Q_{ext} = 2.1281681 Q_{sca} = 1.8074585 Q_{abs} = 0.31770967

MASS EXTINCTION COEF. = 1.6693756 /LAMBDA/DENSITY
then the coated sphere

WHICH PARTICLE TYPE:
1) SPHERE EXACT
2) COATED SPHERE EXACT
3) INFINITE CYLINDER EXACT
4) FINITE CYLINDER 1ST ORDER VARIATIONAL
5) COATED INFINITE CYLINDER EXACT
6) CUBE SEMI-EMPIRICAL
7) OCTAHEDRA SEMI-EMPIRICAL
8) FLAKE SEMI-EMPIRICAL
9) CONVEX-CONCAVE SEMI-EMPIRICAL
10) OTHER IRREGULAR SEMI-EMPIRICAL

INDEX OF REFRACTION FOR COATING $m_1$ & $k_1$ ?
[1.56,0]

INDEX OF REFRACTION FOR CORE $m_2$ & $k_2$ ?
[1.7,7]

(CORE RADIUS)/(COATING RADIUS) = ? (0=CORE RADIUS IS CONSTANT)
[0.215]

WHICH PARTICLE SIZE DISTRIBUTION (MODE# = 1):

1) MONODISPERSED I
2) GATES-GAUDIN-SCHUMANN $x^{(-A)}$
3) LOG-NORMAL $1/(S*G+A)*EXP(-(LOG(X)-LOG(XM))^2/(2*SG**2))$
4) GAMMA $U**(U+1)/(U+1)!*(-R/U/S**(U+1))*EXP(-R/S)$
5) MODIFIED GAMMA $R**A*EXP(-B*R**G)$
6) ROSIN-RAMMLER $X**(N-1)*EXP(-B*X**N)$
7) MULTI-MODAL

DO YOU WANT ANY PART OF THE PHASE FUNCTION (YES=0) ?
[1]

ENTER SIZE PARAMETER FOR COATING
[5.928]

QEXT= 2.5299668 QSCA= 2.3888416 QABS= 0.1411519
MASS EXTINCTION COEF.= 2.0111575 /LAMDA/DENSITY

Thus we have $\omega = .85$ for the carbon-water case and $\omega = .94$ for the carbon nucleated case. Clearly it is the carbon nucleated case which will defeat the seeker while the carbon-water mixture is just on the threshold.
Example 3

If a 1 km wide cloud is produced with carbon fibres chopped to block a 94 GHz (3-mm) signal (i.e. length=1.5mm) and has a concentration of 1 mg/m³, will the signal be blocked and can a naked eye observer see through it? Assume that the fibres have a radius of 1 μm and index of refraction of 1.7 - .7i in the visible and are perfectly conducting at 94 GHz.

For 94 GHz signal, the finite fibre model must be used with $L = \pi \approx 3.14159$ and radius size parameter $x = .0021$. Since the fibres are perfectly conducting the index of refraction must be very large, so we will take $m = 10^9 - 10^3i$. For the visible case we will take $\lambda = .5\mu m$ and therefore $L = 1.88 \times 10^4$ and $x = 12.57$. Since $L \gg 200$ the infinite cylinder case can be used. The calculation then proceeds as follows:

WHICH PARTICLE TYPE:
1) SPHERE EXACT
2) COATED SPHERE EXACT
3) INFINITE CYLINDER EXACT
4) FINITE CYLINDER 1ST ORDER VARIATIONAL
5) COATED INFINITE CYLINDER EXACT
6) CUBE SEMI-EMPIRICAL
7) OCTAHEDRA SEMI-EMPIRICAL
8) FLAKE SEMI-EMPIRICAL
9) CONVEX-CONCAVE SEMI-EMPIRICAL
10) OTHER IRREGULAR SEMI-EMPIRICAL

INDEX OF REFRACTION $m & k$?
[1.E9,1.E9]
RADIUS SIZE PARAMETER?
[.0021]

WHICH PARTICLE SIZE DISTRIBUTION (MODE# = 1):
1) MONODISPERSED $I$
2) GATES-GAUDIN-SCHUMANN $I^{(-A)}$
3) LOG-NORMAL $1/(S+I)*\exp(-(\log(I)-\log(XM))^2/(2*SG^2))$
4) GAMMA $U^{(U+1)}/(U+1)!*(R+U/S+(U+1))!*exp(-U+R/S)$
5) MODIFIED GAMMA $R^A*exp(-B*R^G)$
6) ROSIN-RAMMLER $X^{(N-1)}*\exp(-B*X^N)$
7) MULTI-MODAL

DO YOU WANT ANY PART OF THE PHASE FUNCTION (YES=O)?

ENTER PARTICLE SIZE OR LENGTH PARAMETER
[3.14159]

ORIENTATION ANGLE (O=RANDOM)?

IS CYLINDER RADIUS "<.6 MICRONS" (O=YES)

24
The important output, in both cases, is the mass extinction coefficient. With the density of carbon being typically about 2 g/cm³, we get $\alpha = 165.8$ at 94 GHz and $\alpha = 354$ for the human observer. From equation (4) we can now calculate $T_{94\text{GHz}} < 10^{-7}$ and
Thus the signal is blocked but the human easily sees through the cloud.
Example 4

As a last example we want to show that large water drops will produce first and second order rainbows, scatter sunlight predominantly forward and produce a glory (which one sees while in an aircraft around the shadow of the airplane). Assume that the raindrops are distributed according to

\[ F(z) = z^6 e^{-0.042z}. \]

This distribution is the modified gamma function (9) with \( \alpha = 6, b = 0.042 \) and \( \gamma = 1 \). The peak of the distribution is at about \( z = 213 \) or about 18.6\( \mu \text{m} \) and the effective particle size is about 28\( \mu \text{m} \). All particle sizes from \( x = 0 \) to \( x = 500 \) will be considered. With \( \lambda = 0.55\mu \text{m} \) the calculation is thus:

**WHICH PARTICLE TYPE:**
1) SPHERE EXACT
2) COATED SPHERE EXACT
3) INFINITE CYLINDER EXACT
4) FINITE CYLINDER 1ST ORDER VARIATIONAL
5) COATED INFINITE CYLINDER EXACT
6) CUBE SEMI-EMPIRICAL
7) OCTAHEDRA SEMI-EMPIRICAL
8) FLAKE SEMI-EMPIRICAL
9) CONVEX-CONCAVE SEMI-EMPIRICAL
10) OTHER IRREGULAR SEMI-EMPIRICAL

**INDEX OF REFRACTION** \( m & k ? \)

\[ [1.33,0] \]

**WHICH PARTICLE SIZE DISTRIBUTION (MODE= 1):**

1) MONODISPERSED I
2) GATES-GAUDIN-SCHUMANN \( x^{(-A)} \)
3) LOG-NORMAL \( 1/(SG*X)*EXP(-(LOG(X)-LOG(XM))^2/(2*SG^2)) \)
4) GAMMA \( U^{(U+1)/(U+1)!}*(R**(U/S)**(U+1))*EXP(-U*R/S) \)
5) MODIFIED GAMMA \( R**A*EXP(-B*R**G) \)
6) ROSIN-RAMMLER \( X**(N-1)*EXP(-B*X**N) \)
7) MULTI-MODAL

**INPUT STEP SIZE IN INTEGRATION OVER SIZE DISTRIBUTION**

\[ 1 \]

**LOWER AND UPPER LIMITS OF PSD (BETWEEN 0 AND 499.90)**

\[ [0,500] \]

**INPUT A,B,G**

\[ [6, 0.042, 1] \]

**DO YOU WANT ANY PART OF THE PHASE FUNCTION (YES=O)?**
ENTER LOWEST, HIGHEST AND INCREMENT OF ANGLES IN PHASE FUNCTION
[0, 180, 1]

WHICH POLARIZATION STATE? 1) PARALLEL
2) PERPENDICULAR
OR 3) RANDOM

WITH RESPECT TO SCATTERING PLANE.

DO YOU WANT TO SEE PSD? (O=YES)

Note that an integration step size of 1 was used. This is probably adequate for this example but for distributions that do not cover such a wide range of sizes much smaller step sizes are recommended. A diagram of the phase function is given (not directly obtainable from this program!) since 181 different angles were asked for giving too large a listing of numbers to print here. From the diagram it is seen that most of the light will be scattered in the forward direction or near 0°. The first and second order rainbow are the peaks at about 137° and 129° respectively. The enhancement near and at 180° gives the glory.
1st and 2nd order rainbow

Example 4
APPENDIX B

Errors Found in References

In this appendix the errors found in the texts and literature used in developing the codes for the scattering program are indicated. They do not need to be known for successfully running the code. They are presented here for completeness and, if necessary to aid in any future modification of the code. As the notation used here is the same as in the respective references most of the explanations here should be read with consultation with the original references. This should cause little problems since all references are readily available from the MRL library.

Sphere

No errors found in Kerker (1969) for the Mie routine or Abramowitz and Stegun (1964) for the Bessel functions.

Coated Sphere

No errors found in Bohren and Huffman (1983) in the text. However, the code found in Appendix B was found to have serious numerical instabilities when the real part of the refractive index was less than 1. Furthermore, special cases could be found where ANCAP and BNCAP became infinite. A simple adjustment of the branching condition, found in this part of the program, cured these problems.

Infinite Cylinder

Kerker (1969) was used for the writing of this code. Two errors were found. First, equation (6.1.33) should be divided by $A$. The second error is found only in some printings. This occurs in the sum in equations (6.1.30) and (6.1.31) which should contain $\sin(n\theta)$ and not $\cos(n\theta)$. Again the prescription to obtain the integer order Bessel functions, from Abramowitz and Stegun (1964), were found to be error free.

Coated Infinite Cylinder

The reference used for this code was Ruck (1970). There are three equations in error that can be corrected, by the inclusion in the appropriate places, by one term. Thus if $E$ represents the error term then equations (4.2-66) to (4.2-68) should read

$$C_{n}^{TM} = -\frac{V_{n}P_{n} - Eq_{n}^{2}J_{n}(x_{o})H_{n}^{(1)}(x_{o})}{p_{n}N_{n} - E[q_{n}H_{n}^{(1)}(x_{o})]^{2}},$$

29
\[ C_n^{TE} = - \frac{M_n N_n}{P_n N_n} E \frac{q_n^2 J_n(x_o) H_n^{(1)}(x_o)}{\gamma_n H_n^{(1)}(x_o)} \]
and

\[ C_n = i^{\frac{1}{2}} \frac{E x_o q_n}{\pi x_o P_n N_n} - E |q_n H_n^{(1)}(x_o)|^2 \]

where

\[ E = Z_n Y_n / s_o^2. \]

**Finite Cylinder**

The series of papers Pederson et al (1984,1985) and Waterman (1984) were used as well as Tai (1951). In the papers of Pederson et al, the formulation for the complete solution is given. It remains, however, to perform several analytic integrations. Two of these integrations are difficult but the solution of these integrals can be found in Tai (1951). Unfortunately, they both are missing a term. The term to be added to the integral is \( \cos^2 x \cos^2 q x L4x. \) And a similar term should be added to the integral being \( \sin^2 x \sin^2 q x L4x. \) These corrections can be found in Bowman et al (1987).

The calculation of the sine and cosine integrals followed the simple schemes in Abramowitz and Stegun (1964) again without error.

**Irregular Particles**

No significant errors were found in Pollack and Cuzzi (1979) from where this code is derived.
APPENDIX C

Programs and Subroutines Used

Here are listed all the programs and subroutines that are used in making the execution file 1PHASE.

Irregular and Root

<table>
<thead>
<tr>
<th>Program</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1PHASE</td>
<td>Interactive plus Irregular Shapes</td>
</tr>
<tr>
<td>MIE</td>
<td>Mie component of Irregular shapes</td>
</tr>
</tbody>
</table>

Sphere

<table>
<thead>
<tr>
<th>Program</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SPHEREPHASE</td>
<td>Polydispersions</td>
</tr>
<tr>
<td>MIEPHASE</td>
<td>Double precision Mie routine</td>
</tr>
</tbody>
</table>

Coated Sphere

<table>
<thead>
<tr>
<th>Program</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>COATPHASE</td>
<td>Polydispersions</td>
</tr>
<tr>
<td>COAT</td>
<td>Mie routine</td>
</tr>
</tbody>
</table>

Cylinder

<table>
<thead>
<tr>
<th>Program</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CYLPHASE</td>
<td>Polydispersions</td>
</tr>
<tr>
<td>CYLINDERPHASE</td>
<td>Mie routine</td>
</tr>
<tr>
<td>RANDOMC</td>
<td>Random Orientation</td>
</tr>
</tbody>
</table>

Coated Cylinder

<table>
<thead>
<tr>
<th>Program</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>COATCYLPHASE</td>
<td>Polydispersions</td>
</tr>
<tr>
<td>COATCYL</td>
<td>Mie routine</td>
</tr>
<tr>
<td>RANDOMCC</td>
<td>Random Orientation</td>
</tr>
</tbody>
</table>

Finite Cylinder

<table>
<thead>
<tr>
<th>Program</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>FIBER</td>
<td>Variational routine</td>
</tr>
<tr>
<td>RANDOMF</td>
<td>Random Orientation</td>
</tr>
<tr>
<td>SETUP</td>
<td>Adjust index and impedance</td>
</tr>
<tr>
<td>SC</td>
<td>Sine and Cosine Integral</td>
</tr>
</tbody>
</table>

The above routines have been collected into a library called SCAT so that it is simple to change just one code and obtain 1PHASE. For example if the code FIBER was modified then to create the up-dated version of 1PHASE the following must be typed:

$FORTRAN FIBER
$LIB SCAT FIBER
$LINK 1PHASE,SCAT/LIB

31
An interactive program for estimating extinction and scattering properties of most particulate clouds

An interactive computer program is described that enables the user to calculate the phase function, extinction, scattering and absorption efficiencies, the mass extinction coefficient and backscatter to extinction ratio for most particulate clouds. These clouds may be composed of either mono- or polydispersed particles of the following geometries: sphere, coated sphere, infinite cylinder, coated infinite cylinder, finite cylinder or various irregular shapes. The non-spherical regular shapes may be either oriented or have random orientation.