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CR-83-0100-3

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OSD - 1366

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AD - A133489

MIE CODE AGAUS 82

August 1983

By

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Under Contract DAAG-29-81-D-0100
Contract Monitor: R. C. Shirkey

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REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER ASL-CR-83-0100-3	2. GOVT ACCESSION NO. AD-A133489	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) MIE CODE AGAUS 82		5. TYPE OF REPORT & PERIOD COVERED Final Report
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) August Miller		8. CONTRACT OR GRANT NUMBER(s) DAAG-29-81-D-0100
9. PERFORMING ORGANIZATION NAME AND ADDRESS Battelle Columbus Laboratories Durham, North Carolina		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 1L162111AH71
11. CONTROLLING OFFICE NAME AND ADDRESS US Army Electronics Research and Development Command Adelphi, MD 20783		12. REPORT DATE August 1983
		13. NUMBER OF PAGES 39
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office) US Army Atmospheric Sciences Laboratory White Sands Missile Range, NM 88002		15. SECURITY CLASS. (of this report) UNCLASSIFIED
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE
16. DISTRIBUTION STATEMENT (of this Report) Approved for public release; distribution unlimited.		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)		
18. SUPPLEMENTARY NOTES Contract Monitor: R. C. Shirkey		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) Mie code Phase functions Relative humidity effects Radiative transfer		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) This report contains descriptions of the mathematical background and a user's guide for Program AGAUS, a computer code which performs scalar Mie-based calculations of the single-scattering properties of polydisperse spherical aerosols. The principal quantities calculated by AGAUS are extinction, absorption, scattering and backscattering coefficients, and the angular intensity distribution of unpolarized incident radiation. A number of other quantities,		

20. ABSTRACT (cont)

cont → produced by AGAUS exist and are described in the user's manual portion of this report.(chapter 2).

AGAUS contains internal coding for seven different analytical size-distribution models and permits entry of an "arbitrary" model as discrete data pairs (radius and relative or absolute number density). Provision is made for combining up to five of the analytic models within a single run and for single-run looping over wavelength or certain other aerosol parameters. In addition, AGAUS contains internal coding for taking account of the growth of hygroscopic particles with varying relative humidity.

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CHAPTER 1

MATHEMATICAL OVERVIEW

1.1 Introduction

Program AGAUS treats electromagnetic scattering and absorption of spherical particles by Mie theory. The rigorous formulation of the problem of the interaction of a sphere and a plane wave can be found in a number of books on advanced electromagnetic theory^{1 2 3} and will not be repeated here. In the interest of clarity and uniformity of notation, however, a brief summary of the needed results of the theory is included. The primary objective of this section is to provide descriptions of ways in which AGAUS handles integrations over distributions of particle sizes and mixtures of different particle size-distributions.

In analytic notation, a "size-distribution" (or, a "model") is described by a "distribution function" $f(r)$ with the property that $f(r)dr$ is the relative number of particles (within a unit volume of space) having radii between r and $r + dr$. (In a strict mathematical sense, $f(r)$ is a "probability density function," but the present usage is common.) The total number of particles per unit volume (N) is found by integrating $f(r)dr$ between minimum and maximum values of r appropriate to a given physical situation. Within AGAUS, $f(r)$ has the units "particles per cubic centimeter per micrometer radius."*

1.2 Notations for Individual Particles

Common Mie theory assumes that the interacting sphere is homogeneous and characterized by a radius and a complex index of refraction $n = m - ik$. The overall interaction is usually characterized by quantities called "efficiency factors" represented by the letter Q . Four such quantities are used in AGAUS and are given subscripts e , a , s , and r representing extinction, absorption, scattering, and backscattering, respectively. When multiplied by the geometric area of the sphere, the efficiency factors give cross sections for the above processes. Cross sections are often represented by the letter C , with an appropriate subscript. The Q 's and C 's are functions of the complex index of refraction (itself a function of wavelength) and of the radius of the sphere and the wavelength of incident radiation. Except for the implicit

¹Van de Hulst, 1957, Light Scattering by Spherical Particles, John Wiley and Sons, Inc., New York

²W. K. H. Panofsky and M. Phillips, 1962, Classical Electromagnetic Theory, second edition, Addison-Wesley Publishing Co., Cambridge, MA, pp 233

³M. Born and E. Wolf, 1959, Principles of Optics, Pergamon Press, Oxford, England, pp 630

*With the exception of type 0, within the actual computer code, $f(r)$ is internally normalized in such a way that $N = 1$, and the absolute number of particles per unit volume is determined from data that must be supplied by a user. For this reason, $f(r)$ is called a "relative" number density in chapter 2.

dependence of m and k on the wavelength, the particle radius and wavelength affect the efficiency factors only in ratio form, giving rise to a dimensionless "size parameter" α --the circumference of the sphere divided by the wavelength.

The detailed angular distribution of scattered radiation is described by a "phase function" $p(\Omega)$, which gives the scattered energy per unit solid angle per unit incident radiation. The phase function, like the Q 's, is a function of radius, the wavelength, and the index of refraction. Since problems treated by AGAUS are azimuthally symmetric, p is often written as $p(\theta)$ even though it is properly a function of both θ and ϕ .

1.3 Notations for a Single Size-Distribution Model

In dealing with an aerosol model consisting of many particles of identical composition but varying radii, the efficiency factors (and the phase function) must be weighted by the distribution function $f(r)$ to secure an overall cross section. Thus, for example, the total scattering cross section for all particles in a unit volume of space is given by

$$C_s(\lambda) = \int_{r_{\min}}^{r_{\max}} \pi r^2 Q_s(r, m, k, \lambda) f(r) dr, \quad (1.1)$$

with similar formulae for extinction, etc.

In the same vein, one can define an average cross section per particle (or a cross section per average particle) via

$$\bar{C}_s = C_s(\lambda)/N, \quad (1.2)$$

where N is the number of particles per unit volume. The average phase function $\bar{p}(\theta)$ is found from

$$\bar{p}(\theta) = \frac{1}{N} \int_{r_{\min}}^{r_{\max}} p(\theta) f(r) dr. \quad (1.3)$$

1.4 Mixtures of Size-Distribution Models

To indicate how AGAUS combines mixtures of two or more aerosol models, a subscript i will be added to $f(r)$ and to the Q 's and p . Thus $f_i(r)$ will represent the distribution function for the i th component of a mixture, etc.

Then

$$N_i = \int_{r_{\min}}^{r_{\max}} f_i(r) dr, \quad (1.4)$$

$$C_{S_i}(\lambda) = \int \pi r^2 Q_{S_i}(r, m, k) f_i(r) dr, \quad (1.5)$$

$$\bar{C}_{S_i} = C_{S_i}(\lambda) / N_i, \text{ etc.} \quad (1.6)$$

The total cross sections for a mixture are then found from formulae such as

$$C_S = \sum_i N_i \bar{C}_{S_i} \quad (1.7)$$

The combined phase function is calculated from

$$p(\theta) = \frac{\sum_i N_i \bar{p}_i(\theta) \bar{C}_{S_i}}{\sum_i N_i \bar{C}_{S_i}}, \quad (1.8)$$

so that

$$\int_{\theta} \int_{\phi} p(\Omega) d\Omega = \frac{\lambda^2}{4\pi}. \quad (1.9)$$

Note that the FINAL phase functions printed by AGAUS are normalized such that the above integral is unity.

The detailed relationships between the Q's, $p(\theta)$, and the parameters m , k , and α are summarized in section 1.8.

1.5 Extinction, Scattering, and Radar Coefficients

Readers may note that the "cross sections" discussed above do not really have the usual dimension of area, but rather the dimensions of area per unit

volume, or of inverse length. Thus, for example, C_e represents the extinction cross section for all those particles located in a unit volume of space. Multiplication of C_e by the volume of an optical path is required to get the true extinction cross section for the path. If one assumes a unit cross section for such a path, then C_e can be regarded as an extinction "coefficient" K_e . AGAUS calculates and prints several such "coefficients" having the final unit "per kilometer." As an example, consider a homogeneous path of L kilometers. The optical depth of the path is given by

$$\tau = K_e L , \quad (1.10)$$

and the radiation intensity $I(L)$ would be found from

$$I(L) = I(0) \exp(-\tau) . \quad (1.11)$$

1.6 Treatment of Hygroscopic Particles

Hygroscopic particles absorb water from an ambient atmosphere and may undergo growth to sizes that differ from their initial values. The easiest type of growth to formulate is that in which the absorbed liquid water and the initial material form a solution droplet. Even this simple type of situation is quite complicated, but certain useful approximations do exist and are used in AGAUS. The best known survey of the growth of hygroscopic particles and attendant changes in optical properties is that of G. Hanel,⁴ whose reading is highly recommended for anyone wishing to utilize these features of AGAUS.

The starting point for size adjustments is the equation⁴

$$\left(\frac{r}{r_0}\right)^3 = 1 + \frac{\rho_s \mu(a_w)}{\rho_w} \frac{a_w}{1 - a_w} , \quad (1.12)$$

⁴G. Hanel, 1976, "The Properties of Atmospheric Aerosol Particles as Functions of the Relative Humidity at Thermodynamic Equilibrium with the Surrounding Moist Air," Advances in Geophysics Vol. 19, Academic Press, New York

which is essentially a combined form of equations (2.31) and (2.22) of reference 4. The quantities appearing here are ρ_s , the mass density of the original aerosol material (the solute); ρ_w , the mass density of pure liquid water; μ , Hanel's "growth factor"; and a_w , the "water activity" of the system.

The water activity a_w is related to the equilibrium particle radius r , the fractional humidity f (percent per 100), and the temperature T through the equation

$$a_w = f/e^{\zeta/r}, \quad (1.13)$$

where $\zeta = \frac{2\sigma v}{RT}$,

in which σ is the molecular weight, v is the surface tension, R is the universal gas constant, T is the kelvin temperature.

Equations (1.12) and (1.13) are coupled by r and a_w and are solved simultaneously by means of an iterative procedure.

From equation (1.13)

$$\frac{a_w}{1 - a_w} = \frac{f}{e^{\zeta/r} - f}. \quad (1.14)$$

Substitution of equation (1.14) into (1.12) yields

$$\left(\frac{r}{r_0}\right)^3 = 1 + \frac{\rho_s \mu}{\rho_w} \frac{f}{e^{\zeta/r} - f}. \quad (1.15)$$

Equation (1.15) is then used as follows: an initial estimate of r is taken to be the dry radius r_0 and is used to calculate the right-hand side of the equation. This procedure provides a new value of r via the equality. The new value is then used to recalculate the right-hand side of equation (1.15) to get a second estimate of r . This procedure is continued until a new estimate differs from the previous one by no more than 0.01 percent.

"G. Hanel, 1976, "The Properties of Atmospheric Aerosol Particles as Functions of the Relative Humidity at Thermodynamic Equilibrium with the Surrounding Moist Air," Advances in Geophysics, Vol 19, Academic Press, New York

After exit from the iteration procedure, equation (1.13) is then used to calculate a value for a_w . The net droplet density is then found from

$$\rho = \rho_s \left(1 + \frac{\mu a_w}{1 - a_w} \right) / A, \quad (1.16)$$

where

$$A = 1 + \frac{\rho_s}{\rho_w} \cdot \frac{\mu f}{e^{\zeta/r} - f} \quad (1.17)$$

Equations (1.16) and (1.17) are essentially equation (2.46) of reference 4.

The complex index of refraction $n = m - ik$ is then obtained from

$$m = m_w + (m_s - m_w) / A, \quad (1.18)$$

and

$$k = k_w + (k_s - k_w) / A. \quad (1.19)$$

Since the growth factor μ is generally a function of a_w , the procedure outlined above is not truly complete. A user must still supply a value for μ in some fashion. As a matter of fact, μ may even be an indirect function of radius, but Hanel states that it is reasonable to use an average value $\bar{\mu}$ and to ignore that complexity.

Perhaps the easiest way to enter a value of μ into AGAUS is via the input parameter EMUA ($\bar{\mu}$ —assumed to represent an averaged value as noted above) and to ignore the dependence of μ on r . EMUA must still be regarded as a function of a_w (or the fractional humidity), however. The only reliable way to determine the appropriate values of $\bar{\mu}$ for a given material is by experimental measurements. Reference 4 provides some guidance in the matter as well as some examples of $\bar{\mu} - f$ dependencies for several aerosol models.

⁴G. Hanel, 1976, "The Properties of Atmospheric Aerosol Particles as Functions of the Relative Humidity at Thermodynamic Equilibrium with the Surrounding Moist Air," Advances in Geophysics, Vol 19, Academic Press, New York

1.7 Validation of AGAUS

The continued fraction subroutine (MIEGX), which does the actual Mie calculations in AGAUS, was evaluated by Burlbaw and Miller⁵ through comparisons with J. V. Dave's routine DAMIE.⁶ In all cases for which the latter routine was considered to be reliable (size parameters to 400 for nonabsorbing spheres, and smaller size parameters for absorbing spheres), the agreements were to five digits or better. MIEGX was also tested against a code MIE2, developed by Radiation Research Associates, and again showed equally good agreement. Unlike most other known codes, MIEGX does not fail at the machine level (that is, does not produce underflows or overflows arising from finite precision "roundoffs," etc) even at size parameters of 1000 or greater (see also section 2.2.3).

The halving method of integration employed in AGAUS has been validated by comparing the results of complete runs for several different aerosol models with results published by others, including Shettle and Fenn⁷ and Deirmendjian.⁸ Some of these evaluations have been reproduced in reference 5. Any users who wish to make similar evaluations should remember principles of the halving method* and should be sure to make the convergence criterion (delta) small enough to insure that the minimum interval in radius is comparable to that used by others.

1.8 Summary of Mie Theory Used in AGAUS

Mie theory predicts the scattering by and the absorption in an isolated, discrete, homogeneous, isotropic sphere of radius r with a known complex refractive index $n = m - ik$ relative to the surrounding medium and illuminated by monochromatic radiant energy with wavelength λ in the surrounding medium. The theory is given in detail in standard texts and need not be repeated here. Instead, those elements of theory needed for an understanding of the numerical algorithms used are included. The information in this section is partially based on material from Burlbaw and Miller⁵ and Shirkey et al.⁹

⁵E. Burlbaw and A. Miller, 1981, Modification of Single Scattering Model AGAUSX, ASL-CR-0780-1, US Army Atmospheric Sciences Laboratory, White Sands Missile Range, NM

⁶J. V. Dave, 1972, Development of Programs for Computing Characteristics of Ultraviolet Radiation, Technical Report for Contract NAS5-21860 (NASA), IBM Corporation

⁷E. P. Shettle and R. W. Fenn, 1979, Models for the Aerosols of the Lower Atmosphere and Effects of Humidity Variations on their Optical Properties, AFGL-TR-79-0214, Air Force Geophysics Laboratory, Hanscomb Field, MA

⁸D. Deirmendjian, 1969, Electromagnetic Scattering on Spherical Polydispersions, American Elsevier Publishing Company, Inc, New York

*See section 1.10.

⁹R. C. Shirkey et al, 1980, Single Scattering Code AGAUSX: Theory, Applications, and Listing, ASL-TR-0062, US Army Atmospheric Sciences Laboratory, White Sands Missile Range, NM

All scattering properties of spheres are computed from m and k , and through the use of the induced electric and magnetic multipole moments of the sphere a_ℓ and b_ℓ , respectively. The moments are given by*

$$a_\ell = \frac{\Psi'_\ell(n\alpha) \Psi_\ell(\alpha) - n \Psi_\ell(n\alpha) \Psi'_\ell(\alpha)}{\Psi'_\ell(n\alpha) \xi_\ell(\alpha) - n \Psi_\ell(n\alpha) \xi'_\ell(\alpha)}, \quad (1.20)$$

and

$$b_\ell = \frac{n \Psi'_\ell(n\alpha) \Psi_\ell(\alpha) - \Psi_\ell(n\alpha) \Psi'_\ell(\alpha)}{n \Psi'_\ell(n\alpha) \xi_\ell(\alpha) - \Psi_\ell(n\alpha) \xi'_\ell(\alpha)}. \quad (1.21)$$

The prime denotes differentiation with respect to the argument. The $\Psi_\ell(z)$ and $\xi_\ell(z)$ functions are Ricatti-Bessel functions of the first and third kinds, respectively, and are related to spherical Bessel functions $j_\ell(z)$ and $n_\ell(z)$ by

$$\Psi_\ell(z) = z j_\ell(z), \quad (1.22)$$

and

$$\xi_\ell(z) = z j_\ell(z) - i z n_\ell(z) = \Psi_\ell(z) + i \chi_\ell(z), \quad (1.23)$$

where

$$j_\ell(z) = \left(\frac{\pi}{2z}\right)^{1/2} J_{\ell+1/2}(z), \quad (1.24)$$

* α is the Mie size parameter and is equal to $2\pi r/\lambda$, where r is the radius of a sphere.

and

$$n_\ell(z) = \left(\frac{\pi}{2z}\right)^{1/2} N_{\ell+1/2}(z) . \quad (1.25)$$

The function $J_{\ell+1/2}(z)$ is the half integral order Bessel function; the function $N_{\ell+1/2}(z)$ is the half integral order Neuman function.

The extinction cross section is computed from

$$C_{\text{ext}} = \frac{\lambda^2}{2\pi} \sum_{\ell=1}^{\infty} (2\ell + 1) \text{Re}(a_\ell + b_\ell) , \quad (1.26)$$

and the scattering cross section from

$$C_{\text{sca}} = \frac{\lambda^2}{2\pi} \sum_{\ell=1}^{\infty} (2\ell + 1) [|a_\ell|^2 + |b_\ell|^2] . \quad (1.27)$$

The various cross sections are the basic quantities used in scattering problems, but they are not the quantities usually computed directly from Mie algorithms. Instead, it is more convenient to compute dimensionless efficiency factors Q_{ext} and Q_{sca} , which depend on m , k , and α , and which are multiplied by the geometrical sphere cross section to obtain the true cross section $C_j = \pi r^2 Q_j$. Thus,

$$Q_{\text{ext}} = \frac{2}{\alpha^2} \sum_{\ell=1}^{\infty} (2\ell + 1) \text{Re}(a_\ell + b_\ell) , \quad (1.28)$$

and

$$Q_{\text{sca}} = \frac{2}{\alpha^2} \sum_{\ell=1}^{\infty} (2\ell + 1) [|a_\ell|^2 + |b_\ell|^2] . \quad (1.29)$$

Although the cross sections account for the energy removed from the forward beam, they do not give any information about where the scattered photons go. This information is contained in scattering amplitudes and intensity factors that relate the flux density scattered through an angle θ relative to the incident flux density. There are two amplitudes, $S_1(\theta)$ and $S_2(\theta)$, and intensity factors $i_1(\theta)$ and $i_2(\theta)$, which correspond to light, respectively, polarized perpendicular and parallel to the plane of scattering defined by the direction of incidence and the direction of scattering.

The intensity factors are related to the scattering amplitudes by

$$i_1(\theta) = |S_1(\theta)|^2, \quad (1.30)$$

$$i_2(\theta) = |S_2(\theta)|^2. \quad (1.31)$$

The amplitudes come from the multipole moments through

$$S_1(\theta) = \sum_{\ell=1}^{\infty} \frac{2\ell + 1}{\ell(\ell + 1)} [a_{\ell}\pi_{\ell}(\theta) + b_{\ell}\tau_{\ell}(\theta)], \quad (1.32)$$

and

$$S_2(\theta) = \sum_{\ell=1}^{\infty} \frac{2\ell + 1}{\ell(\ell + 1)} [b_{\ell}\pi_{\ell}(\theta) + a_{\ell}\tau_{\ell}(\theta)], \quad (1.33)$$

and angular factors $\pi_{\ell}(\theta)$ and $\tau_{\ell}(\theta)$ defined in terms of associated Legendre functions:

$$\pi_{\ell}(\theta) = P_{\ell}^1(\cos \theta)/\sin \theta, \quad (1.34)$$

$$\tau_{\ell}(\theta) = \frac{dP_{\ell}^1(\cos \theta)}{d\theta}. \quad (1.35)$$

Alternative expressions frequently used are

$$\pi_{\ell}(\theta) = \frac{dP_{\ell}(\cos \theta)}{d(\cos \theta)}, \quad (1.36)$$

and

$$\pi_{\ell}(\theta) = \cos \theta \cdot \pi_{\ell}(\theta) - \sin^2 \theta \cdot \frac{d\pi_{\ell}(\theta)}{d(\cos \theta)}, \quad (1.37)$$

where

$$P_{\ell}(\cos \theta) = \frac{1}{2^{\ell} \ell!} \frac{d^{\ell}}{d(\cos^{\ell} \theta)} (\cos^2 \theta - 1)^{\ell}. \quad (1.38)$$

These functions satisfy the following recurrence relations:

$$\pi_{\ell}(\theta) = \cos \theta \frac{(2\ell - 1)}{(\ell - 1)} \pi_{\ell-1}(\theta) - \frac{\ell}{\ell - 1} \pi_{\ell-2}(\theta), \quad (1.39)$$

and

$$\tau_{\ell}(\theta) = \cos \theta [\pi_{\ell}(\theta) - \pi_{\ell-2}(\theta)] - (2\ell - 1) \sin^2 \theta \pi_{\ell-1}(\theta) + \pi_{\ell-2}(\theta). \quad (1.40)$$

The scattering cross section measures the ability of a particle to scatter light; consequently, C_{sca} is expected to be obtained from an integral over the scattering intensity factors. Equation (1.27) follows from

$$C_{\text{sca}} = \frac{\lambda^2}{4\pi} \int_{-1}^1 (i_1(\theta) + i_2(\theta)) d(\cos \theta). \quad (1.41)$$

Although the intensity factors themselves may be used in scattering calculations, they are primarily suited for computing flux densities, and frequently scattered light can be more conveniently measured and computed in terms of radiances. Radiances do not have an inverse square distance dependence; therefore, the distance from the scatterer to the detector need not be known if the detector field of view is small and is filled by the scattering cloud. The phase function $p(\theta)$ gives a radiance I scattered into the θ direction in terms of the radiance I_0 incident on the particle.

The phase function is dimensionless and is defined in AGAUS as

$$p(\theta) = \frac{\lambda^2}{8\pi^2 C_{sca}} [i_1(\theta) + i_2(\theta)] . \quad (1.42)$$

The integral of the final normalized phase function printed by AGAUS is unity.

For the special case of $\theta = 180^\circ$, backscatter, the efficiency is expressed by the radar cross section σ . The radar cross section may be defined as 4π times the backscattered power per steradian divided by the incident power per unit area or

$$\sigma = 4\pi r^2 I(r, 180^\circ) / I_0 . \quad (1.43)$$

This expression can be reduced by the relations

$$I(r, \theta) = \frac{I_0 \{i_1(\theta) + i_2(\theta)\}}{2k^2 r^2} \quad (1.44)$$

and

$$i_1(180^\circ) = i_2(180^\circ) = |S_1(180^\circ)|^2 . \quad (1.45)$$

Thus

$$\sigma = \frac{4\pi}{k^2} |S_1(180^\circ)|^2 , \quad (1.46)$$

and when divided by the geometrical cross section, $G = \pi r^2$,

$$Q_{\text{radar}} = \frac{\sigma}{G} = \frac{4|S_1(180^\circ)|^2}{\sigma^2}, \quad (1.47)$$

where $\alpha = 2\pi r/\lambda$. Using

$$-\pi_\ell(180^\circ) = \tau_\ell(180^\circ) = (-1)^\ell \cdot \frac{1}{2} \ell (\ell + 1), \quad (1.48)$$

one obtains

$$-S_1(180^\circ) = S_2(180^\circ) = \sum_{\ell=1}^{\infty} \left(\ell + \frac{1}{2}\right) (-1)^\ell (a_\ell - b_\ell). \quad (1.49)$$

1.9 Numerical Techniques for Mie Theory in AGAUS

Most of the numerical calculations performed by AGAUS are those associated with calculating the coefficients a_ℓ and b_ℓ . These calculations are performed by a subroutine (MIEGX) that is based on a "continued-fraction" method for finding the Ricatti-Bessel functions. The method employed is that of W. J. Lentz.¹⁰ This method was chosen because it provides very good accuracy using only single-precision arithmetic and because of the ease with which it handles large size-parameters and imaginary parts of the complex index of refraction. Since the method is not widely employed, it is reviewed in some detail here.

Subroutine MIEGX used in AGAUS is a modified version of a routine (DAMIE) originally developed by J. V. Dave.⁶ The major modification, made by Lentz,¹⁰ was the use of a continued-fraction method rather than ordinary backward recursion techniques for evaluating some of the quantities appearing in equations (1.20) and (1.21). The continued-fraction method will be discussed in more detail below. It is noted, at this point, however, that the angular functions π_ℓ and τ_ℓ are evaluated in MIEGX using forward recursion and

¹⁰W. J. Lentz, 1976, "Generating Bessel Functions in Mie Scattering Calculations using Continued Fractions," Appl Opt, 15(3):668

⁶J. V. Dave, 1972, Development of Programs for Computing Characteristics of Ultraviolet Radiation, Technical Report for Contract NAS5-21860 (NASA), IBM Corporation

equations (1.39) and (1.40) and starting values $\tau_0(\theta) = 0$, $\pi_1(\theta) = 1$, $\tau_0(\theta) = 0$, and $\tau_1(\theta) = \cos \theta$.

For computational purposes of MIEGX, equations (1.20) and (1.21) may be rewritten in the following forms:⁶

$$a_\ell = \frac{\left[\frac{A_\ell(n\alpha)}{n} + \frac{\ell}{\alpha} \right] \operatorname{Re}[\xi_\ell(\alpha)] - \operatorname{Re}[\xi_{\ell-1}(\alpha)]}{\left[\frac{A_\ell(n\alpha)}{n} + \frac{\ell}{\alpha} \right] \xi_\ell(\alpha) - \xi_{\ell-1}(\alpha)}, \quad (1.50)$$

$$b_\ell = \frac{\left[nA_\ell(n\alpha) + \frac{\ell}{\alpha} \right] \operatorname{Re}[\xi_\ell(\alpha)] - \operatorname{Re}[\xi_{\ell-1}(\alpha)]}{\left[nA_\ell(n\alpha) + \frac{\ell}{\alpha} \right] \xi_\ell(\alpha) - \xi_{\ell-1}(\alpha)}, \quad (1.51)$$

where

$$A_\ell(z) = -\frac{\ell}{z} + \frac{J_{\ell-1}(z)}{J_\ell(z)}, \quad (1.52)$$

and $z = n\alpha$ is complex.

Several methods have been used for evaluating the quantities ξ_ℓ and A_ℓ . The principal difference between MIEGX and Dave's Mie routines is the way in which the ratios A_ℓ are found. Lentz's continued-fraction method evaluates the quantities A_ℓ . A brief summary of the latter method is given below, but interested readers should refer to Lentz's article for detailed information.

To simplify notation, the common form for a continued fraction:

⁶J. V. Dave, 1972, Development of Programs for Computing Characteristics of Ultraviolet Radiation, Technical Report for Contract NAS5-21860 (NASA), IBM Corporation

$$f = g_1 + \frac{1}{g_2 + \frac{1}{g_3 + \frac{1}{g_4 + \frac{1}{g_5 + \dots}}}} \quad (1.54)$$

will be written as

$$f = g_1 \oplus \frac{1}{g_2} \oplus \frac{1}{g_3} \oplus \frac{1}{g_4} + \dots \quad (1.55)$$

With the first of those notations, Lentz showed that

$$\frac{J_{\ell-1}(z)}{J_{\ell}(z)} = \frac{2\ell}{z} \ominus \frac{1}{(\ell+1)z^{-1}} \oplus \frac{1}{2(\ell+2)z^{-1}} \ominus \frac{1}{2(\ell+3)z^{-1}} + \dots \quad (1.56)$$

To clarify the procedure used in MIEGX, it is most convenient to use a second compacted notation for the continued fraction (1.54):

$$f = [g_1, g_2, g_3, \dots] \quad (1.57)$$

Then, defining the "kth convergent" to be

$$f_k = [g_1, g_2, g_3, \dots, g_k] \quad (1.58)$$

Lentz showed that

$$f_k = \frac{[g_1] \dots [g_{k-1}, \dots, g_1] [g_k, \dots, g_1]}{[g_2] \dots [g_{k-1}, \dots, g_2] [g_k, \dots, g_2]} \quad (1.59)$$

The order of the terms appearing in equation (1.59) has been reversed to emphasize that the evaluation begins with g_1 rather than with an unknown value g_k .

The ratio $J_{\ell-1}(z)/J_{\ell}(z)$ can now be expressed in the form of equation (1.59) if one takes

$$g_i = (-1)^{i+1} 2(\ell + i + 1) z^{-1} \quad (1.60)$$

Subroutine MIEGX utilizes the foregoing procedures for calculation of the ratios $J_{\ell-1}/J_{\ell}$ needed to evaluate the Mie coefficients a_{ℓ} and b_{ℓ} . In practice, MIEGX initially determines the value of A_{ℓ} and some value of ℓ , say $\ell = N$, such that N is the largest value of ℓ whose use is expected in a particular run. The required $J_{\ell-1}/J_{\ell}$ ratio is evaluated by calculating the relevant value of f_k [equation (1.59)] for a sequence of k values up to the k for which

$$|f_k - 1| < \epsilon, \quad (1.61)$$

where ϵ is a tolerance value corresponding to the precision available within a particular computer. ϵ is given the value of 10^{-6} for 32-bit precision calculations.

Once A_N has been found,* the values of A_{ℓ} for $\ell < N$ are found by backward recursion and are stored in an array for recall as needed in evaluating the Mie summations of

$$\text{Re}[S_1(\theta)], \text{Im}[S_1(\theta)], \text{Re}[S_2(\theta)] \text{ and } \text{Im}[S_2(\theta)].$$

The sum is terminated when

*If N exceeds the dimension NDIM of the complex array $A(\)$, MIEGX, then $A_{2 \times \text{NDIM}}$ (or $A_{3 \times \text{NDIM}}$, etc.) is calculated and backward recursion is used to

find the needed A_{ℓ} 's.

$$|a_l|^2 + |b_l|^2 < \epsilon \quad (1.62)$$

and when the fractional change in the radar efficiency is also less than ϵ , that is, when

$$\left| \frac{Q_{\text{rad } l} - Q_{\text{rad } l-1}}{Q_{\text{rad } l}} \right| < \epsilon . \quad (1.63)$$

This is more stringent than the first test alone and is a test on the phase functions as well.

For size parameters smaller than 0.01, the cumbersome Mie apparatus is bypassed and Van de Hulst's¹ analytic approximations are used for finding the efficiency factors and phase function.

MIEGX returns the following quantities as required by AGAUS: Q_{ext} , Q_{sca} , Q_{rad} , and $P(J)$. The $P(J)$ as returned by MIEGX are average intensities and must be further normalized to become the actual phase functions [equation (1.42)]. Some limitations associated with numerical implementation of the above procedures are discussed in section 2.2.3.

1.10 Other Numerical Procedures Used in AGAUS

AGAUS handles numerical integrations of the type indicated in equations (1.3) and (1.5) using the "trapezoidal rule" and a process called "halving." The latter process is described next.

A general idea of how program AGAUS performs integrations over sizes can be obtained by considering a numerical method for determining the area under a curve $g(r)$ versus r such as that sketched in figure 1. The objective is to evaluate numerically an integral

$$G = \int_{r_{\text{min}}}^{r_{\text{max}}} g(r) dr \quad (1.64)$$

¹Van de Hulst, 1957, Light Scattering by Spherical Particles, John Wiley and Sons, Inc., New York

to some desired degree of accuracy using the smallest number of values of r for the numerical calculations. The procedure adopted in AGAUS is as follows (reference to figure 1 may be helpful):

a. An initial estimate G_1 of the value of the integral is made with three values of r labeled by Roman numeral I and the "trapezoidal rule."

b. A second estimate G_2 is then made with increments Δr , which are half as large as those used in getting G_1 . In getting G_2 , the two additional r -values labeled II are utilized.

c. The values of G_2 and G_1 are compared to each other by calculating a quantity

$$\delta = \frac{|G_2 - G_1|}{|G_2|} \quad (1.65)$$

and comparing it to a preset quantity Δ .

If $\delta < \Delta$, then it is assumed that G_2 is a "sufficiently" accurate representation of G , and the computations are terminated. If on the other hand, $\delta > \Delta$, one proceeds.

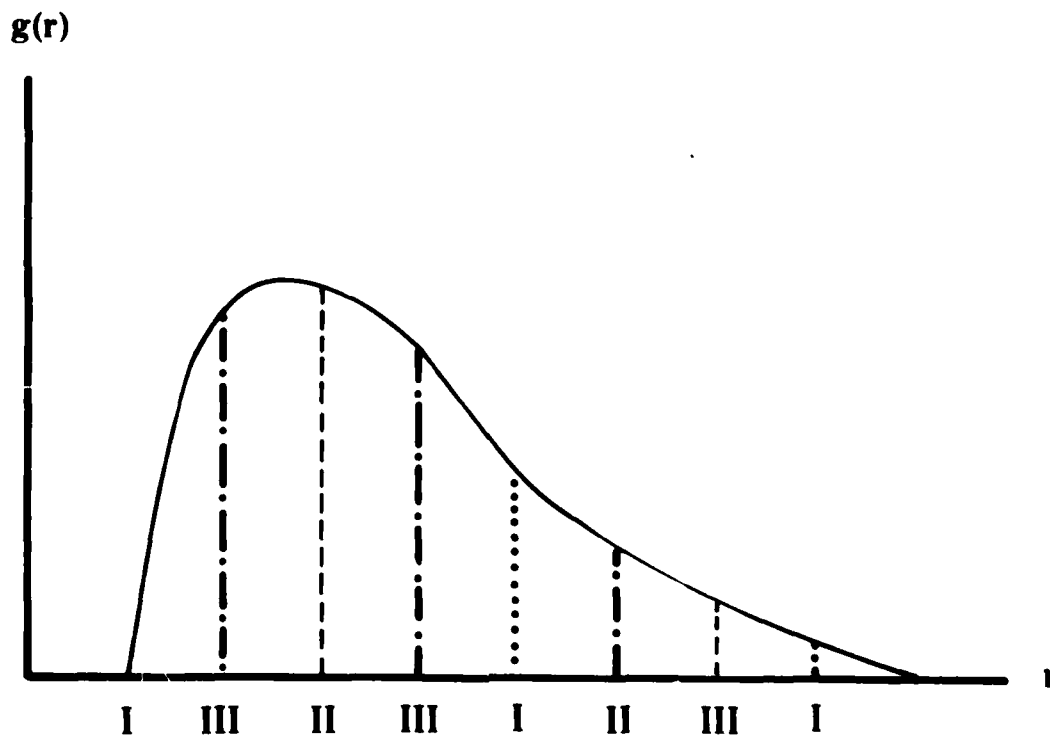


Figure 1. Sketch of how values of particle radii are selected in the halving procedure of AGAUS.

d. A third estimate G_3 of G is then made by again cutting the increment Δr to half its previous value. This results in the addition of computations at the three new r -values labeled III in figure 1. A new value of δ is then calculated from

$$\delta = \frac{|G_3 - G_2|}{G_3} , \quad (1.66)$$

and δ is again compared to Δ . If δ is still greater than Δ , the spacing between r -values is cut in half once more, and the "estimation-comparison" process is repeated until either $\delta < \Delta$ or some maximum number of r -values has been reached.

In AGAUS, the quantity used in the testing process is the total volume of the aerosol particles, namely,

$$V = \int \frac{4}{3} \pi r^3 f(r) dr . \quad (1.67)$$

Volume was chosen as the quantity to be tested because its r^3 dependence might make it converge more slowly than the extinction or scattering cross sections while maintaining a reasonable convergence for phase functions. The code may be easily modified to test on any desired quantity; however, the maximum number of radii allowed by AGAUS depends on the number of size groups defined in a run and may be changed by revision of the source code (see section 2.3.2 for additional discussion of this matter).

CHAPTER 2

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2.1 Introduction

AGAUS is a Mie scattering code for calculation of the single-scattering properties of polydisperse spherical particles. The primary quantities calculated by AGAUS are the extinction, scattering, absorption, and backscatter coefficients plus the angular intensity distribution produced by various forms of particle size-distributions. The code contains seven different size-distribution models and also permits a user to provide an arbitrary size model as a set of discrete numerical input data. There is, in addition, a special subcode that may be used to tabulate the Mie efficiency factors (extinction, scattering, absorption, and backscatter) as a function of particle radius. An important feature of this version of AGAUS is the ability to treat and combine the scattering properties of a mixture of up to five different size-distributions in a single run and to repeat the process for an arbitrarily large number of wavelengths. A method for handling the effect of relative humidity on the equilibrium sizes of hygroscopic particles is also included.

2.2 Summary of Output Quantities

This section presents a summary of the quantities produced and printed in a run of AGAUS. More detailed descriptions may be found in subsequent sections.

2.2.1 Definitions

a. "Size-distribution model" refers to a particular functional relationship between the relative number of particles per unit radius and the values of the radius.

b. "Distribution-type" refers to a number that identifies the various "size-distribution models" that are recognized by AGAUS as valid.

c. "Size-group" or "size-bin" refers to particular ranges of values of particle radii for which certain optical properties are calculated and printed by the program. To clarify what is meant, consider a situation in which one wants to examine particles with radii between 0.0 μm and 10 μm , but would like to see the properties of particles whose radii lie in the ranges 0.0 μm to 2.0 μm , 2.0 μm to 5.0 μm , and 5.0 μm to 10.0 μm . This would be handled by dividing the overall range (0.0 to 10.0) into three "size-groups," with "group 1" belonging to radii between 0.0 μm and 2.0 μm , etc.

2.2.2 Major Outputs

With those definitions the major outputs can now be described:

a. **Particles per Gram.** The number of particles in a 1-g sample of material if all the particles in the sample had radii belonging to a size-group.

b. **Number Fraction.** The ratio of the number of particles that would belong to a size-group to the sum of the numbers of particles in all size-groups being used in a run. As an example, suppose that three size-groups are being used and that a 1-g sample contains 10 particles with sizes belonging to group 1, 100 particles in group 2, and 5 particles in group 3. Then the number fraction for group 1 would be $10/(10 + 100 + 5)$. For group 2 it would be $100/(10 + 100 + 5)$, and so forth.

c. **Mass Fraction.** The fraction of the mass contained by particles in ALL size-groups that would belong to particles whose radii place them in a selected size-group. Continuing the above example, suppose that the 10 particles in group 1 has a mass of 0.0005 g, those in group 2 a mass of 0.80 g, and those in group 3 a mass of 0.1995 g. Then the mass fraction for group 1 would be 0.0005; for group 2, 0.8; and for group 3, 0.1995.

d. **Cumulative Mass Fraction.** The sum of the mass fractions of all size-groups up to and including the group for which this quantity is generated. The cumulative mass fractions for the examples above would then be 0.0005, 0.8005, and 1.0000.

e. **Group Cross Sections in Square Centimeters per Gram.** Extinction, absorption, scattering cross sections that would exist if 1 g of material existed among particles whose radii fell inside a size-group.

f. **Group Cross Sections in Square Centimeters per Particle.** The quantities of the preceding form divided by the number of particles per gram (item 1 above).

g. **Weighted Averages.** (Extinction, absorption, etc.) cross sections as integrated against the relative number of particles per unit radius described by the size-distribution model in use. These results have the units of square centimeters per particle.

h. **Extinction, Scattering, and Backscattering Coefficients.** The weighted averages (item 7, above) multiplied by the total number of particles per cubic centimeter associated with a particular size-model after summation over all size-distribution models being treated in a particular run of AGAUS. The unit of these quantities is "per kilometer," so that the "optical depth" of a transmission path is the product of these "coefficients" and the length of the path in kilometers.

i. **Phase Functions.** The relative intensity per unit solid angle of scattered radiation as a function of angle as averaged over all pertinent size-groups and size-distribution models. The phase functions are normalized so that their integrals over all solid angles are unity.

j. **Attenuation Coefficient.** This quantity gives the total extinction coefficient with units of square meters per milligram of aerosol material to be found in an optical path. The attenuation coefficient may appear with two "suffixes" referring to "dry" and "wet" aerosols. In that context, "dry" means the number of milligrams of aerosol present before any adjustment of particle radii caused by accretion of liquid water arising from the hygroscopic properties of the material. "Wet" means the number of milligrams of the aerosol that would exist after taking hygroscopic properties into

account. In other words, the "wet" attenuation is that which would be expected after the dispersal of 1 mg of a hygroscopic material into an environment whose relative humidity will lead to the accretion of liquid water and an increase in the sizes and masses of the original aerosol particles (that is, when Hanel's growth formulae are invoked).

In addition to the above quantities, AGAUS also provides a printed recapitulation of most of the input data and several other derived results that may be of interest to at least some users. If warranted, certain diagnostic and warning messages are also printed.

2.3 Input data Requirements

Input data for AGAUS are formulated as a set of standard 80-column punched cards or card-images. At least four types of data cards are required for a run. If a user selects certain program options, as many as three additional types of data cards may be needed. Those optional data cards are identified below as card types 3A, 3B, and 3C. Again depending on options selected, some types of cards may need to be repeated to provide additional data such as a new wavelength value.

2.3.1 Card Type 1

This card is required (although it may be blank) and may contain up to 80 alphanumeric characters identifying the run. The format is 40A2.

2.3.2 Card Type 2

This card contains a set of 11 program control parameters entered as integers with the format (11I5). The symbolic names of these parameters and their meanings are described next and must appear on the data card from left to right in the order in which they are given below.

NWAVE NWAVE is nominally the number of wavelengths to be treated within a single run of the program, but may also be used to define the number of times one wishes to loop over any variable found on cards of type 5 (below). NWAVE must be 1 or greater. A minimum of NWAVE cards of type 5 is necessary.

NIDSTP NIDSTP is the number of different size-distribution types to be combined at each wavelength. The maximum value of NIDSTP is 5.

IW IW is a parameter that may be used to indicate that the particles of all size-distribution models are to be treated as though they were composed of liquid water. To select that option, IW should be set to zero. If IW = 0 any values of the complex refractive index and the mass density (specific gravity) found on card type 5 will be ignored and replaced by those of liquid water at the temperature (°C) that is taken from card type 5. To avoid these features, set IW = 1. If IW = 0, the wavelength on data card(s) type 5 must be between 0.2 μ m and 200.0 μ m.

- IDELT** IDELT is used to signal the presence or absence of card 3A from the input data deck. If card type 3A is not to be present, set IDELT to zero. Use IDELT = 1 if card type 3A will be present. If IDELT = 0, default values of the data that may appear on card 3A are defined by the program.
- NANG** Parameter NANG specifies the number of angles at which the phase function is to be calculated. The value of NANG must be between 1 and 65. If phase functions are of no particular interest, set NANG = 1 or 0. The values of the angles used in the calculation will depend on the parameter IANG (next). The value of NANG has a significant effect on running time, so one should use as small a value as is consistent with other needs.
- IANG** IANG is used to choose from among three ways of selecting the angles at which phase functions are calculated. Note, however, that the phase functions are printed only if parameter NANG is 3 or greater.
- IANG = 0 will override the input value of NANG (setting it to 65) and will result in the use of 65 equally spaced angles between 0 and 180 degrees.
- IANG = 1 will recognize the value of NANG as entered and result in the use of NANG equally spaced angles between 0 and 180 degrees.
- IANG = 2 informs the program that cards of type 3B carrying values for the angles to be used will be found in the data deck. This option allows a user to specify whatever set of values for the angles may be desired.
- NBINS** NBINS is, in general, the number of size-groups into which the run is to be subdivided. (NBINS = 0 is an exception discussed later.) The maximum permissible value of NBINS is 50. If NBINS is not zero, a user must supply cards of type 3C in the input data deck. Those cards carry the user's definitions of the radii to be associated with each size-group. An input value of zero for NBINS will provide the use of just one size-group, with the minimum and maximum radii determined either from data entered on cards of type 4 or by the program itself. If NBINS = 0, there must be no data cards of type 3C in the input data deck. Note also that NBINS must be set to zero if use of size-distribution type number zero is selected on a card of type 4 below. (See also section 2.3.2.)
- IEO** Parameter IEO controls the generation of an output data disc or tape file containing several run parameters (below) and the values of the phase functions. If no such file is wanted, be sure to set IEO = 0. There are two other legal choices for the value of IEO:
- IEO = 1 overrides the users values of NANG and IANG and results in the use of 65 predetermined angles for phase function calculations. This option will result in a file compatible with EOSAEL usage.

IEO = 2 also overrides the value IANG on card 2 and sets IANG = 2. The latter means that the user must supply a set of data cards of type 3B carrying NANG values for the angles to be used in the phase function calculations.

In both cases the output file is written on logical unit number NEOU (next parameter). The file will contain the following quantities:

1. The angles, with format (11(F6.2,1X)).
2. The number of angles, a phase function identifier (set to zero by AGAUS, which implies user supplied data for subsequent use as EOSAEL input), the wavelength (micrometers), the albedo for single scattering, and the extinction and scattering coefficients (per kilometer). These items are written with the format (2(I2,1X), F5.2,1X,F8.6,1X,2(E12.6,1X)).
3. The phase functions, written with a format of (6(E12.6,1X)), at the angles noted immediately above. The phase functions are normalized so that their integrals over all solid angles are unity.

NEOU NEOU is the logical unit number to be used to identify the file controlled by IEO. If in doubt, use zero for both IEO and NEOU.

NUNIT If NUNIT is nonzero, the following quantities are written on logical unit number NUNIT for each radius at which Mie calculations are made during a run: dry radius, radius after any increase related to relative humidity, the relative particle number at the dry radius, and the Mie efficiency factors for extinction, scattering and backscatter.

MQRTE Normally zero, but if MQRTE = 12345, the quantities listed under NUNIT will be directed to whatever logical unit has been assigned to the listing device for the run. (That assignment is logical unit number 6 unless altered by changing the value of the parameter IOUT in the COMMON BLOCK subroutine of AGAUS).

2.3.3 Card Types 3A, 3B and 3C

These cards are more or less optional but their presence or absence in a data deck must be properly correlated with the values of the parameters IDELT, IANG, IEO, and NBINS, which appear on card 2.

Card 3A contains two variables: DELTA and ATOP with the format (2E10.4).

DELTA DELTA is the value of the "convergence criterion" used to decide when to terminate the integration over particle sizes within each size-group. The running time of AGAUS is intimately connected to the value of DELTA used in a run. The default value of DELTA (used if IDELT = 0 and card 3A is therefore absent) is 0.001. A value of 0.01 will probably meet most needs if great accuracy is not needed. A value of 0.1 is often adequate for sample or test runs.

ATOP This parameter sets an upper limit to the Mie size-parameter for which complete Mie calculations are done. Its default value is 400. The function of ATOP is the following: whenever a particle radius has a value that corresponds to a size-parameter that is larger than ATOP, the actual value of the size-parameter is ignored and a size-parameter equal to ATOP is used instead. The first time that happens, the results of the Mie calculation are saved and substituted when any subsequent particle's size-parameter exceeds ATOP. This procedure can save computation time and usually does not introduce a significant amount of error in the values of the efficiency factors (and cross sections) because they approach constant values at large size-parameter values. The effect of the approximation is more severe on the phase functions, however, but are not likely to be devastating since the relative number of very large particles is ordinarily small. If ATOP is made larger than 400, inherent numerical behavior of the Mie subroutine may lead to unreliable values of the backscattering efficiency factor and possibly of the phase functions associated with large size-parameters.

The actual value of ATOP at which the above-mentioned instabilities begin to appear is linked to the size of a complex array A() in subroutine MIEGX rather than to a more intrinsic property such as use of single precision arithmetic. Those instabilities first seem to appear when the size parameter being treated reaches a value that is approximately equal to the dimension of the array A. In the standard version of MIEGX, A is defined to contain 400 complex elements or 800 single precision floating point numbers. The choice of 400 rather than 200 or 1000 was made as a compromise between program core requirements and anticipated Mie size parameters found in normal usage. If sufficient memory is available, the dimension of A() may be increased substantially, thereby moving the size parameter at which instabilities might occur to values larger than 400. Test runs have been made with the dimension of A as large as 3000 without the appearance of obvious instabilities of the type under discussion. Users who contemplate increasing the dimension of A() must note that one other parameter (NDIM) would also require a change. This is discussed explicitly in paragraph e of section 2.4.3.

Card(s) 3B carry the angles to be used in the phase function calculations if a user chooses to supply them. These cards carry up to 16 values per card with the format (16F5.1). The symbolic quantity read from these cards is an array labeled ANGL in the source code. The number of entries should be equal to the value of NANG placed on card 2. There must be no extra cards: for NANG between 1 and 16, use one card; for NANG between 17 and 32, use two cards, etc.

Card(s) 3C are used to supply the upper radius limit for the size-groups, which are read under the format (8E10.4). The symbolic quantities on this type of card are labeled RR (a 51-element array) in the FORTRAN source code. The values of the RR's must be in ascending order, and the first entry should be the upper limit in radius for the first size-group. (The lower limit on radius for the first size group is normally zero if these cards are used at all, that is, if NBINS is nonzero). There must be at least NBINS entries, and

no extra cards are permitted. There must of course be enough cards to make the number of data values equal to NBINS. Remember that NBINS must not be greater than 50.

2.3.4 Card Type 4

Type 4 cards carry the data that select the size-distribution model (or models) to be assumed for a run and certain parameters associated with the different models. Up to five cards of this type are permitted for most runs (exception is type 0; see below). The number of cards of this type that are required is specified by the value of NIDSTP on card 2.

All cards (except some cards for model IDSTP = 0; see below) have the general form:

IDSTP, Q1, Q2, Q3, Q4, Q4, Q6

The format is (I3,7X,6E10.4) and in all cases IDSTP is an integer that identifies a "distribution-type." It must be placed in column 3. The Q's have different interpretations for different distribution-types and will be given symbolic names in the ensuing lines.

2.3.4.1 Type 0. Arbitrary User-Supplied Discrete Model. This distribution-type allows a user to enter from 1 to 513 pairs of data (one pair per card) for the value of a particle radius and an absolute number of particles having that radius. This model is selected by using a type 4 data card containing a zero in column 3 and the number of data pairs as a floating point number in columns 11-20. In other words, Q1 (above) on the first type 4 card should be the number of data pairs to be expected by the program. Note that this particular distribution type requires an absolute number density.

A user must then insert NRADI data cards each carrying a value of radius (in micrometers) and an absolute number density (in particles per cubic centimeter per micrometer), where NRADI is the number of radius values to be used. The format is (2E10.4).

Users should probably not try to mix a type 0 model with some other type under the NIDSTP greater than 1 option. Such mixtures have not been tested.

2.3.4.2 Type 1. Lognormal Distribution

IDSTP, RLO, RHI, RBAR, SIGMA, DENS

Q1 is RLO - The minimum radius at which the model is to be cutoff.

Q2 is RHI - The maximum radius at which the model is to be cutoff.

Q3 is RBAR - The radius at which the relative number density peaks.

Q4 is SIGMA - The standard deviation to be used (Not LN(SIGMA)).

Q5 is DENS - The number of particles per cubic centimeter.

This distribution has the mathematical form:

$$f(r) = \frac{C}{r} \exp \left\{ -\frac{1}{2} \left[\frac{|\ln(r/r_0)|}{\ln(\sigma)} \right]^2 \right\} \quad (2.1)$$

where $f(r) dr$ is the relative number of particles with radii between r and $r + dr$, and C is a normalization constant.

RLO and RHI are, in a sense, optional: if RLO = RHI, then the code will itself assign cutoff values (that is, will redefine both) that insure that most of the particle radii will be included in the calculation. To select that option just make the values of Q1 and Q2 equal to zero. Note, however, that they must not be omitted: RBAR, SIGMA, and DENS must still be in positions Q3, Q4, and Q5. This option relative to RLO and RHI is not valid for the other distribution types (below).

DENS is also optional but only in a sense. If a user does not want to specify the number density, entering a value of 0.0 will tell the program to calculate the number density from the mass density (RHOA, card 5), the mass concentration (CONC, card 5) and the (computed) average volume per particle. If both DENS and CONC are zero, the program assigns a default value DENS = 1.0. This behavior of DENS is also applicable to the other distribution types (listed below) that also use DENS as an input parameter.

2.3.4.3 Type 2. Double Exponential Model

IDSTP, RLO, RHI, Q, A, B, DENS

RLO, RHI, and DENS have the same meaning as listed under type 1.

The meanings of A, B, and Q are best described by the mathematical form for the distribution:

$$f(r) = Qe^{-A/r} + (1 - Q)e^{-B/r} \quad (2.2)$$

(In the FORTRAN source code Q has the symbolic name CUE.)

2.3.4.4 Type 3. Power Law Model

IDSTP, RLO, RHI, Q, A, DENS

The form of the distribution is

$$f(r) = Qr^{-A} \quad (2.3)$$

RHO, RHI, and DENS are again (in fact, are always) defined as in type 1 above.

2.3.4.5 Type 4. Hoidale Dust Model

IDSTP, VIS

VIS is the visibility in kilometers.

This is a model of type 3 in which RLO is 0.1, RHI = 15.0, Q = 30.0, and A = 4.0. For this particular model, the value of DENS is found from the relationship

$$\text{DENS} = 11.0 ** [5.0 - \text{ALOG10}(\text{VIS})] . \quad (2.4)$$

2.3.4.6 Type 5. Modified Gamma Distribution

IDSTP, RLO, RHI, RC, ALF, GAM, DENS

The form of the distribution is

$$f(r)dr = r_c r^\alpha \exp\left\{-\frac{\alpha}{r} \left(\frac{r}{r_c}\right)^\gamma\right\} . \quad (2.5)$$

r_c (that is, RC) is the mode radius (at which $f(r)$ peaks); ALF and GAM are user-supplied parameters. Note that parameters for this distribution found in the literature may provide a parameter "b" rather than r_c . The relationship between b and r_c is

$$b = \alpha / (\gamma r_c^\gamma) \quad (2.6)$$

2.3.4.7 Type 6. Modified Gamma Fog Model

IDSTP, RLO, RHI, RC, ALF, GAM, ELWC

The form of this model is the same as in type 5. This model always assumes that the aerosol material will be liquid water droplets and finds the value of DENS from the value of ELWC. ELWC itself is the "liquid water content" in units of grams per cubic meter. Use of this model relieves a user from the need to specify the optical constants (EMA and CAYA, card 5) and the mass density (RHOA, card 5) and an internal table lookup procedure provides those data for water. The tables of Hale and Query (Applied Optics, 12:555, ff) are used in this procedure.

2.3.4.8 Type 7. Special Table Generation Mode. This is not actually a distribution model at all, but is an operating model used for calculating and printing tables of Mie efficiency factors as a function of radius. The input data are as follows:

IDSTP, RLO, RHI, DELR

RLO is the minimum particle radius to be used.

RHI is the maximum particle radius to be used.

DELR is the increment in radius to be used.

This "distribution-model," like all the others, will expect the user to provide the wavelength and the optical constants at each wavelength on data card type 5.

The quantities that are printed are the adjusted (per Hanel) radius, the dry radius, the corresponding Mie size-parameter, the efficiency factors for extinction, scattering, absorption and backscatter, and the adjusted (again per Hanel) index of refraction. The program formats 50 sets of results per page.

This "mode" may be used to generate several sets of tables in a single run, but doing so requires a nonstandard way of arranging the input data cards of types 4 and 5. NWAIVE on card type 2 should be 1; NIDSTP (card 1) should be equal to the number of "sets" for the run (but no greater than 5); NIDSTP pairs of data cards of types 4 and 5 must be "interleaved" rather than collected together as distinct groups of NIDSTP type 4 cards followed by NWAIVE type 5 cards.

2.3.4.9 Type 8. Marshall-Palmer Rain Model

IDSTP, RAIN

RAIN is the rainrate in millimeters per hour.

The form for $f(r)$ is

$$f(r) = Ae^{-Br} , \quad (2.7)$$

with $A = 1.6E-5$ and $B = 8.2E-4 * (RAIN ** (-0.21))$. The value of DENS is found from $DENS = A/B$, which is theoretically valid only if $RLO = 0$ and $RHI = \text{infinity}$. In practice the distribution is cutoff at $RLO = 0.0001$ and $RHI = 2500.0$ (micrometers), but this should induce no appreciable error in DENS since few rain drops will exceed 2.5 mm in radius.

A few words of caution may be helpful in connection with use of this model. The maximum Mie size-parameter used is roughly 13,000 divided

by the wavelength. Since the Mie subroutine used in AGAUS becomes unreliable at size-parameters of the order of 400 to 1000 (depending on which quantities are of most interest), the model is only useful at fairly large wavelengths and is intended for use at wavelengths of the order of 1 mm or so. Because the data tables for optical constants for water do not extend beyond 200 μ m, use of the Marshall-Palmer model is generally inconsistent with setting IW = 0 on data card 2, and users must provide the appropriate optical constants on cards of type 5 (below).

2.3.4.10 Type 9. Hybrid Lognormal and Power-Law Model

IDSTP, RBAR, SIGMA, RMIN, RMAX, PWR

This model consists of the lognormal model (type 1) for radii between zero and RMIN and a power-law (type 3) model for radii between RMIN and RMAX. The number density functions $f(r)$ are made equal at the radius defined by the value of RMIN.

RBAR and SIGMA have the same definitions as in type 1.

PWR is the same quantity as A in type 3.

If either RBAR or SIGMA is zero, this model becomes the same as type 3, with RLO = RMIN and RHI = RMAX. If RMIN and RMAX are equal, then the model is the same as type 1.

One restriction imposed by computer exponent limits is known to exist for the hybrid model, namely that RMIN, RBAR, and SIGMA must be such that the quantity

$$\left| \frac{\ln(RMIN/RBAR)}{\ln(SIGMA)} \right| < 13 .$$

2.3.5 Card(s) Type 5

Cards of this type carry data describing the wavelength to be used and the general physical properties of the aerosol materials whose relative number distributions are specified by cards of type 4. At least one of the type 5 cards is required for each run of AGAUS. More generally the number of type 5 cards needed is given by the product of NWAVE and NIDSTP. The format of type 5 cards is (8E10.4). The symbolic names for the data are:

WAVE, EMA, CAYA, RHOA, CONC, RELHUM, TEMP, EMUA

WAVE - the wavelength in micrometers

EMA - the real part of the index of refraction of the aerosol

CAYA - the absolute value of the imaginary part of the index of refraction

RHOA - the mass density (specific gravity) of the aerosol in grams per cubic centimeter

CONC - the mass concentration (grams of aerosol material per cubic centimeter of space)

RELHUM - the relative humidity in percent

TEMP - the environmental temperature in Celsius degrees

EMUA - Hanel's growth factor " μ -bar"

One card of this type must be supplied for each value of NWAVE and for each value of IDSTP at each wavelength, regardless of the value of IW on card 2.

2.4 Additional Program Information

2.4.1 Choosing Values for DELTA

As was stated under the description for data card type 3, DELTA controls the exit from the numerical integration routine in which the efficiency factors are converted to cross sections and weighted by the relative number density, etc. The integration is done using the trapezoidal rule in a series of steps called "halvings." Each size-group is treated separately. On the first pass across a size-group, computations are done at the endpoints and midpoint of the range of radii belonging to the group. In addition to the cross sections, weighted sums of the phase functions and the total volume of the particles are computed. The program then calculates new estimates of all the above quantities by performing the computations at radii that lie halfway between the radii used in the first pass and combines the newest results to form new estimates of the integrals. After the first two passes, five values of radius will have been used. The program then proceeds through a series of loops in which the spacing of the radii is made half those used in the most recent pass. At the end of each pass (after the second), the most recent value for the integrated particle volume is compared to the one that existed at the end of the previous pass. Exit from this procedure occurs as soon as the difference between the "new" and "old" values for volume divided by the "new" value is less than DELTA. If this criterion is not satisfied after some preset number of "halvings" have occurred, the program exits anyway and prints a message to the effect that convergence was not achieved in treating that particular interval. The number of radii used before automatic exit is determined by an internal program variable NHALV (accessible in the source code but not as a normal input parameter), and its value is dependent on the number of size-groups being treated in a given run.

The maximum number of radii used for each size-group is as follows:

If NBINS is 0, 1, or 2, 513 radii may be used before exit.

If NBINS is 3 or 4, only 257 radii per group are allowed.

If NBINS is 5 or larger, 129 radii are allowed per size-group.

These assignments can be changed in the source code's main program if more or fewer radii are desired, except for the type zero model. Models other than type zero calculate the new radius values as needed, but type zero sets a maximum of 513 radii and places those values in an array for recall. This procedure is used because the user supplied type zero data are unlikely to be spaced at the correct values of radius required by the halving process and an interpolation is made from the user supplied values of the radii to those needed for the halving procedure. Users who have ample memory available could increase the value of 513 to 1025, 2049, etc., by redefining the dimensions of the arrays R(), F(), and FFF() in the source code and recoding a portion of the interpolation procedure. If this process is contemplated, pay particular attention to the parameter NHALV: the maximum number of radii must be equal to $1 + (2 \text{ raised to the power } NHALV)$.

The running time of the program is mainly set by the number of times the Mie subroutine is called and the values of the size-parameters in use; therefore, the use of a very small value of DELTA will force the program to utilize the maximum allowed number of radii for each size-group. The number of radii used might well be far greater than that needed for acceptable precision in the results and hence make the run require an excessive amount of time. The situation is most critical when the number of size-groups is fairly large. In many cases the overall contributions of the particles in some size-groups to the total extinction may be negligible because of the small relative number of particles in those groups, and use of a very small value of DELTA can result in a considerable amount of computation time for large particles that often do not really affect the results very much. The program does not (with one type of exception) make any judgments: the same value of DELTA is used for all size-groups. The exception is as follows: in runs with NBINS greater than zero, the program finds a quantity called VMAX for each size-distribution model in use. This parameter consists of the total particle volume (weighted by occurrence frequency) of particles for whatever size-group makes that quantity a maximum for the whole range of groups in use. VMAX is used in the integration loops discussed above in such a way that an automatic exit from computations for a size group will occur if the volume estimated for the first 33 choices of radius is less than $VMAX * 1.E-6$. This procedure can easily be disabled, if a user so desires, by removing a single line from the source code for subroutine AGXP2. The line in question is one that reads `IF(N.GT.5.AND.VOLHHT.LT.VMAX)GOTO ...`

Suggested values for DELTA are in the range 0.01 to 0.001. If after choosing values of DELTA in this range, the program outputs look "strange" or appear to be questionable, then a rerun with a smaller value of DELTA may be advisable. Users who have not previously used AGAUS should, perhaps, do a little experimenting with a few different values of DELTA to see how its value affects their results.

For distribution type zero (arbitrary, user-supplied model), the suggested value of DELTA is 0.001 or smaller because the interpolations used in that model can present problems if DELTA is not fairly small.

2.4.2 Selecting Values for NBINS and the Size-Group Radius Limits

In many instances, users will not really care to subdivide the range of radii to be used in a run into more than one size-group. In such cases, it will probably be sufficient to set the parameter NBINS = 0, and to control the maximum and minimum cutoff radii via the parameters RLO and RHI on data cards of type 4 (or, for IDSTP = 9, via RMAX). Some situations have arisen, however, in which choosing NBINS greater than zero is advisable even though the breakdown of outputs by size-groups is not particularly wanted. An example of such a situation is one in which the NIDSTP > 0 option is being invoked to treat a bimodal (NIDSTP = 2) or multimodal model in which the distributions that are being combined peak at different values of radius. In that kind of situation, it is advisable to break the computation range into intervals that are roughly centered on the radii at which the various modes have their peaks. Doing that will help the user in being assured that enough points are treated for each mode to make the convergence checks meaningful.

To clarify this state of affairs, consider an aerosol model being described by the lognormal distribution IDSTP = 1, with the first mode being peaked at $r = 0.05\mu\text{m}$ and a standard deviation of about 1.5. Suppose the other mode peaks at $5.0\mu\text{m}$ and has a standard deviation of 2.0. To assure coverage of the major part of the second mode, one would probably choose RLO to be something of the order of 0.001 and RHI to be of the order of 100. Now, a run with NBINS = 0 permits a maximum of 513 radii to be used in the Mie calculations and integrations over sizes. The increment between adjacent radii (if all allowed radii are used in the halving process) is $(\text{RHI}-\text{RLO})/513$, or about $0.2\mu\text{m}$. This increment is far too large to give adequate attention to the mode centered at $0.05\mu\text{m}$. Hence, the first mode might well be virtually ignored in the run. What one needs to do is to make sure that quite a few radii will be chosen to span each peak, and the simplest way to do that is to use the technique suggested above. A more complicated way would be to go into the source code and change the value of the variable NHALV to a larger value. The number of radii chosen between RLO and RHI if NBINS = 0 is $1 + 2^{**}\text{NHALV}$. Making such a change is feasible if the kind of situation discussed is common for a particular user, but it can exact a heavy time penalty by causing the program to utilize an unnecessarily large number of very large Mie size-parameters.

2.4.3 Subsidiary Program Outputs

a. For all distribution types, the program prints a quantity labelled "AVERAGE NUMERICAL DRY VOLUME PER PARTICLE." This quantity is used, when appropriate, to calculate the particle number density DENS.

b. For a few distribution types the program also prints a quantity labelled "AVERAGE ANALYTIC DRY VOLUME PER PARTICLE." This quantity can be determined through formal integration for some of the distribution types and represents the result of an analytic integration over the radii between 0 and infinity. Its value may be meaningful in some situations: if, for example, RLO and RHI were intended to span virtually all particles, a comparison of the "analytic" and "numerical" average volumes per particle give at least a useful indicator of how well that was accomplished. If the two results, when available, differ appreciably it might be advisable to think about whether the values of RLO and RHI are really appropriate for that model.

c. Near the end of the program, the "TOTAL NUMBER OF RADII USED WAS" is printed. The number printed represents the sum of the numbers of radii at which Mie calculations were done, with all size-groups included. Its value may be helpful in selecting a value for DELTA, but it is printed mainly for general interest.

d. After printing the values of the phase functions (which is omitted if parameter NANG is less than 3), the phrase "TEST INTEGRAL OF PHASE-FUNCTION" followed by a number is printed. If the phase functions produced by the run are to be used as input to some subsequent program that will perform numerical integrations involving the phase functions, that number should always be compared to unity. If its value is appreciably different from unity, it is inadvisable to attempt to use the phase functions in later integrations. The discrepancy is a good measure of whether or not enough angles were used in the run to provide adequate accuracy for numerical integrations. Whenever such subsequent integrations are intended, set NANG to the maximum possible value (65 in the standard AGAUS code). If 65 angles still do not produce good agreement between the result printed by the program (that is, a number very near 1.0), a user may be forced to resort to use of a more sophisticated numerical procedure than the trapezoidal method used in AGAUS for this test integration.

e. On occasion, one may find the message "UPPER MIE SIZE LIMIT EXCEEDED IN INTERVAL NO." ... This message indicates that at least one value of particle radius being used for the indicated size-group was so large that the corresponding Mie size-parameter was larger than ATOP. This message is in the nature of a warning, but there may be no action one can take to alleviate the limitation unless ATOP was set below 400. On the other hand, if sufficient addressable memory is available, the array A(400) and the parameter NDIM in subroutine MIEGX can be increased substantially. Experience with MIEGX has generally indicated that "numerical instabilities" (which were mentioned in the discussion of input data card type 3A) occur when the value of a size-parameter exceeds the size of the array A and the parameter NDIM of MIEGX. (The code attempts to compensate for such an occurrence, so the program will not ordinarily abort as one might suspect.) Values of NDIM as large as several thousand have proved usable on systems that can provide the needed array space. The principal "problem" that has been found with MIEGX for size-parameters larger than NDIM has been unreliable values for the backscatter efficiency factor (and by inference, the phase functions at large angles). If those quantities are of no interest, ATOP can be set to almost any (large) value and the extinction and scattering cross sections may be quite reasonable. Users can test this for themselves by exercising the MQRTE = 12345 option (or by running model 7) and examining the behavior of the efficiency factors as a function of radius or size-parameter. The extinction and scattering efficiency factors should behave smoothly and approach the value of 2.0 for very large size-parameters. The smooth behavior is also expected for the backscatter (radar) efficiency factors for large size-parameters. A look at the values of the latter may demonstrate the "problem" under discussion here.

f. Certain anticipated error conditions also generate output statements aimed at making the source of error reasonably visible to the user. In most cases these errors are deemed "fatal" and the run is terminated.

2.5 The NWAWE Looping Options

AGAUS permits looping over any parameter that appears on data card type 5 (see section 2.3.5) if an appropriate input data set is prepared. This section discusses one possible application of this option. Suppose that one wishes to examine the way in which the extinction coefficient of a particular hygroscopic aerosol model changes with relative humidity, and that data for EMUA ($\bar{\pi}(f)$) are available for five values of the relative humidity. One would then set parameter NWAWE = 5 on data card number 2 and prepare cards of types 3 and 4 in the usual way. The choice NWAWE = 5 means that at least five of the type 5 data cards are needed--one for each value of the relative humidity (RELHUM). These five cards would ordinarily carry identical data for parameters WAVE, EMA, CAYA, RHOA, CONC, and TEMP, but different values of RELHUM and EMUA. The value of EMUA on a given card should, of course, correspond to the value of RELHUM on that card.

The use of five type 5 cards to handle five values of RELHUM assumes that only one size-distribution is in use (that is, that NIDSTP = 1). If NIDSTP is greater than 1, the required number of type 5 cards is given by the product of NWAWE and NIDSTP. As an example, suppose that NWAWE = 5 and NIDSTP = 2.

There must then be ten of the type 5 data cards arranged as follows:

```

WAVE, EMA1, CAYA1, RHOA1, CONC1, RELHUM1, TEMP, EMUA11
WAVE, EMA2, CAYA2, RHOA2, CONC2, RELHUM1, TEMP, EMUA12
WAVE, EMA1, CAYA1, RHOA1, CONC1, RELHUM2, TEMP, EMUA21
WAVE, EMA2, CAYA2, RHOA2, CONC2, RELHUM2, TEMP, EMUA22
      :
WAVE, EMA1, CAYA1, RHOA1, CONC1, RELHUM5, TEMP, EMUA51
WAVE, EMA2, CAYA2, RHOA2, CONC2, RELHUM5, TEMP, EMUA52

```

where

EMA_i, CAYA_i are the optical constants for (dry) aerosol component i at wavelength WAVE and temperature TEMP,

RHOA_i, CONC_i are the mass density and mass concentration for component i,

RELHUM_j is the jth value of relative humidity,

and

EMUA_{ij} is the value of $\bar{\pi}(f)$ for aerosol component i at relative humidity value RELHUM_j.

In this example, parameters WAVE, EMA_i , $CAYA_i$, $RHOA_i$, $CONC_i$ and TEMP are held constant, with only RELHUM_j and EMUA_j changing from card to card. One could set up a data deck for looping over any other parameter on the type 5 cards in a similar fashion if desired: use (N WAVE) x (N IDSTP) type 5 cards with all parameters fixed except the one over which looping is to occur. Note, however, that AGAUS does not "remember" any of the parameters, so valid values of WAVE, EMA, etc., must appear on every individual card. There is only one exception to this rule: If IW = 0 (water only case), then the values of EMA and CAYA will be found from the internal tables; any input value, including blanks, will be ignored.

2.6 Differences between AGAUS 82 and Previous Versions

The structure of AGAUS 82 differs in several ways from that of the version listed in reference 9. The principal differences are summarized here for the possible benefit of users of the previous version.

a. The ability to "loop" over a mixture of size-distribution models has replaced the loop over several components (of varying optical properties) having a fixed size-distribution model. Each component now requires definition of a separate size-distribution model even if several components are to be given the same size-distribution model. This option is not available for the "arbitrary" (IDSTP = 0) model.

b. Several new output quantities have been added with breakdowns into particle size groups. These include quantities such as the number of particles per gram and cross sections in square centimeters per gram.

c. The normalization of the phase functions has been changed so that their integral over all solid angle should yield unity.

d. The algorithms for handling the growth and variations in optical properties of hygroscopic aerosols as functions of relative humidity have been replaced by somewhat more sophisticated ones.

e. The original Mie subroutine MIEGX has been replaced by one using different numerical methods and is valid for larger size-parameters than the previous version.

f. Unweighted integrations of extinction coefficients, phase functions, etc., over wavelength have been deleted, and the limit of 10 wavelengths per run has also been deleted.

g. Some of the IEO options have been omitted.

h. All intrinsic "bimodal" size-distribution models have been deleted, as has the one labelled "Deirmendjian's Model." Bimodal cases can now be treated by using the looping option mentioned as item a above. A new

⁹D. Deirmendjian, 1969, Electromagnetic Scattering on Spherical Polydispersions, American Elsevier Publishing Company, Inc., New York

nybrid lognormal/power-law size-distribution model has been added, and a special "model" (IDSTP = 7) has been added to print tabulations of Mie efficiency factors.

i. The option for generating Gauss-Legendre expansion coefficients for the phase function has been removed as has the use of special angles associated with that option.

j. A new input parameter (ATOP) allows users to set an upper limit on the Mie size-parameters to be used in a run.

k. The ordering of the input data cards and the data belonging to each "type" of card have been changed substantially.

l. A new subroutine (DISTR) handles the calculation of the distribution functions $f(r)$ for all cases except the arbitrary (IDSTP = 0) case. Use of this routine makes possible removal of the upper limit of 513 radii per wavelength (except for IDSTP = 0 cases).

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