01 Jan 1976

Mie Scattering Computations For Moderately Large Spherical Particles

Dwight C. Look
Missouri University of Science and Technology, look@mst.edu

Recommended Citation

D. C. Look, "Mie Scattering Computations For Moderately Large Spherical Particles," *Journal of Colloid And Interface Science*, vol. 56, no. 2, pp. 386 - 387, Elsevier, Jan 1976.
The definitive version is available at https://doi.org/10.1016/0021-9797(76)90267-8

Mie Scattering Computations for Moderately Large Spherical Particles[1]

There are several books currently available which describe Mie scattering (1–5). While perusing these books, as well as periodicals, the general feeling is that with the aid of a digital computer any of the quantities of usual interest can be easily computed. The number of terms required for a solution to converge depends on the size parameter; that is, the number of terms, n, required to obtain a solution is slightly more than the size parameter, x. This size parameter depends directly upon the radius of the spherical particle:

$$x = 2\pi a/\lambda \qquad [1]$$

in which a is the radius of the particle and λ is the wavelength of the monochromatic electromagnetic radiation being coherently (or elastically) scattered. Thus, when the particle radius is many times larger than the wavelength, i.e., moderately large; $50 \leq x \leq 400$, the number of terms, n, needed for solution can be quite large ($60 \leq n \leq 450$).

The quantities of interest determined by the Mie scattering formulas consist of infinite series. With finite computer storage, evaluation of these quantities must be limited to some finite number of terms. In practice, the computations of such quantities is made by summing successive terms until the next term alters the sum by some predetermined, arbitrarily small amount. This series truncation requirement may drastically effect the number of terms used (for a given size parameter). It is the purpose of this note to set forth in a little more detail the dependence of a given size parameter and the truncation requirement on the number of terms used as an accurate solution for moderately sized spherical scatterers.

The basic computational problem in determining most of the quantities of interest using the Mie formulas is the evaluation of the a_n and b_n, the so-called Mie coefficients. These quantities are defined as

$$a_n = \frac{[(A_n(y)/m) + (n/x)] \operatorname{Re}\{\zeta_n(x)\} - \operatorname{Re}\{\zeta_{n-1}(x)\}}{\{[A_n(y)/m] + (n/x)\}\zeta_n(x) - \zeta_{n-1}(x)} \qquad [2]$$

$$b_n = \frac{[mA_n(y) + (n/x)] \operatorname{Re}\{\zeta_n(x)\} - \operatorname{Re}\{\zeta_{n-1}(x)\}}{[mA_n(y) + (n/x)]\zeta_n(x) - \zeta_{n-1}(x)} \qquad [3]$$

in which $A_n(y) = \psi_n'/\psi_n(y)$.

The term "Re" implies the "real part" and

$$\psi_n(y) = (\pi y/2)^{\frac{1}{2}} J_{n+\frac{1}{2}}(y)$$
$$\zeta_n(y) = (\pi y/2)^{\frac{1}{2}}[J_{n+\frac{1}{2}}(y) + i(-I)^n J_{-n-\frac{1}{2}}(y)]. \qquad [4]$$

In Eqs. [2], [3], and [4], J_n represents the Bessel function, and $y = mx$ (m is the index of refraction and may be complex). In order to generate $\zeta_n(x)$, the following recurrence relations are used:

$$\zeta_n(x) = \frac{2n-1}{x}\zeta_{n-1}(x) - \zeta_{n-2}(x)$$
$$\zeta_0(x) = \sin x + i \cos x$$
$$\zeta_{-1}(x) = \cos x - i \sin x, \qquad [5]$$

and for $A_n(y)$

$$A_n(y) = -\frac{n}{y} + \left(\frac{n}{y} - A_{n-1}(y)\right)^{-1}$$
$$A_0(y) = \cos y/\sin y. \qquad [6]$$

By using Eqs. [5] and [6], the values of a_n and b_n can be determined directly without using unwieldy Bessel functions. These quantities are the basic parameters needed for the evaluation of the scattering and extinction efficiencies:

$$Q_{\text{sca}} = (2/x^2) \sum_{n=1}^{\infty} (2n+1)[|a_n|^2 + |b_n|^2]$$

$$Q_{\text{ext}} = (2/x^2) \sum_{n=1}^{\infty} (2n+1) \operatorname{Re}(a_n + b_n), \qquad [7]$$

The above equations were programmed for an IBM 360 digital computer, using double precision. Excellent agreement between the results of this program and the data in (5–7) was obtained.

The primary goal of the present study was to determine the effect an impressed truncation requirement had on the number of terms used as a convergent solution for a given size parameter. Following the suggestion of Deirmendjian *et al.* (9), the number of terms used as a solution was determined by the condition

$$\frac{|a_n|^2 + |b_n|^2}{n} \leq C \qquad [8]$$

in which C was varied from 10^{-7} to 10^{-15}. Figures 1 a–c present a portion of the results of the study as a size parameter versus the number of terms. The three

[1] Work presented was supported in part by a National Science Foundation grant NSF ENG 74 22107.

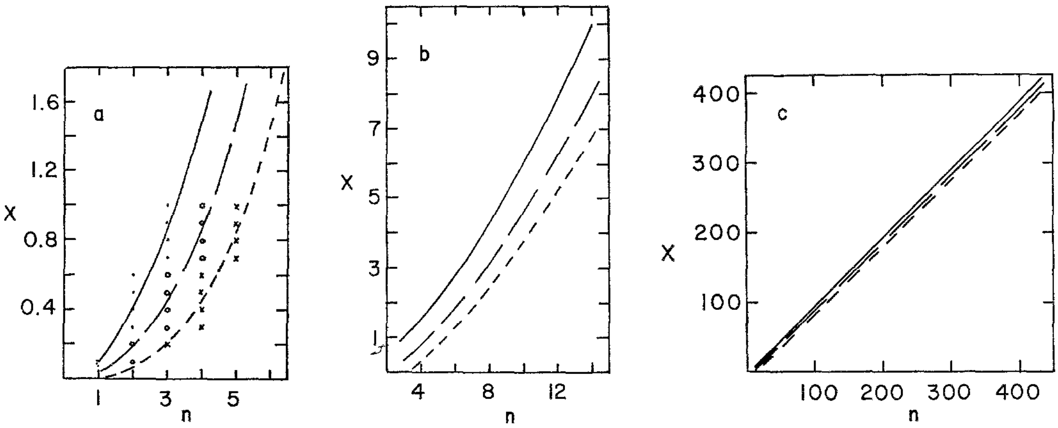

FIG. 1. Size parameter, x, versus the number of terms for convergent solution, n, with C as a parameter: solid line, $C = 10^{-7}$; broken line, $C = 10^{-11}$; and dashed line, $C = 10^{-15}$. (a) small size parameter region $(\cdots)$ represents the range of size parameters with the same number of terms for $C = 10^{-7}$, (ooo) represents size range for $C = 10^{-11}$, and (xxx) represents size range for $C = 10^{-15}$. (b) intermediate size parameters region. (c) moderately large size parameters region.

curves presented are for the cases of $C = 10^{-7}$, 10^{-11}, and 10^{-15}. The complex index of refraction, $m = n' - ik$, was varied such that $1.1 \leq n' \leq 1.6$ and $0 \leq k \leq 1.8$. The curves are independent of the values of n' and k that were used but do depend upon the size of the truncation requirement.

When compiling the data, some errors were noted. For moderately sized values of the imaginary portion of the index of refraction, as the size parameter increased an instability developed in the computed efficiencies. In fact, at some values of x, the efficiency for scatter is greater than the efficiency for extinction. These obviously incorrect results are due to the forward recursion errors in the procedure used.

A closer investigation of this phenomenon yielded the results presented as Fig. 2. Values of x and k in the region below the curves yield acceptable solutions (i.e., no instabilities were noted), whereas values of x and k in the region above the curves yield unacceptable solutions. The truncation requirement for these computations was 10^{-13}. Notice that these curves depend on the real as well as the imaginary part of the index of refraction.

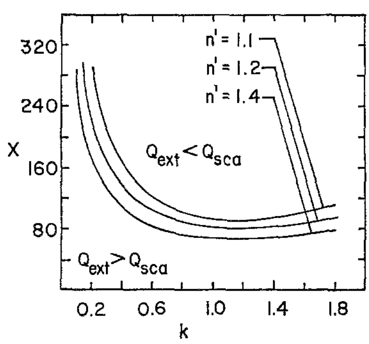

FIG. 2. Size parameter, x, versus the imaginary portion of the index of refraction, k, with the real portion of the index of refraction, n, as parameter.

REFERENCES

1. VAN DE HULST, H. C., "Light Scattering by Small Particles," Wiley, New York, London, 1957.
2. GOODY, R. M., "Atmospheric Radiation I: Theoretical Basis," Oxford at the Clarendon Press, 1964.
3. DEIRMENDJIAN, D., "Electromagnetic Scattering on Spherical Polydispersions," American Elsevier, New York, 1969.
4. KERKER, M., "The Scattering of Light," Academic Press, New York, 1969.
5. WICKRAMASINGHE, N. C., "Light Scattering Functions for Small Particles," Wiley, New York, 1973.
6. GUMPRECHT, R. B. AND SLIEPCEVICH, C. M., "Light Scattering Functions for Spherical Particles," McGraw–Hill Co., New York, 1961.
7. BROCKES, A., *Optik* **21**, 550 (1964).
8. DEIRMENDJIAN, D., CLASEN, R., AND VIEZEE, W., *J. Opt. Soc.* *51*(6), 620 (1961 June).

D. C. LOOK

Radiation Heat Transfer Group
Department of Mechanical and Aerospace Engineering,
University of Missouri, Rolla,
Rolla, Missouri 65401

Received November 10, 1975; accepted January 14, 1976.