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Improved algorithm of light scattering by a coated sphere

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Abstract

An efficient numerical algorithm for computing the light scattering by a coated sphere is proposed. The calculation of relevant functions by different recurrence algorithms is discussed. The new algorithm avoids the numerical difficulties, which give rise to significant errors encountered in practice by prior methods. Exemplifying results such as extinction efficiency, scattering efficiency, light scattering intensity as well as calculation speed are provided. The results show that this algorithm is efficient, fast, numerically stable and accurate.

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1. Introduction

Many technical problems involving small spheres are encountered in various applications (Wang, 2000) as modern technology develops and advances, for instance, the combustion of pulverized coal particles coated with either water or liquid fuel in furnaces and the stabilization of polymer solutions by coating the polymer particles with surfactants. By coating with spheres of special refractive index stealth aircraft can be manufactured. The coated spheres can also incorporate the properties of other materials. In biomedicine polymer chains anchored on a sphere of inorganic material may serve as drug-delivery agents to target some specific location of the body. Furthermore, study of the light scattering and absorption properties of white blood cell (as a model for coated sphere) can reveal the concentration, size distribution and other information of the cell to provide theoretic direction to the design of hemanalysis iatrical apparatus (Choi, 2001; He & Pan, 1997). Research of the properties of light scattering by a coated sphere is therefore worthy of discussion. Such study calls for the calculation of related physical quantities such as scattering intensity, extinction efficiency, scattering efficiency, absorbing efficiency, etc. The key to solve the problem is to calculate the Mie coefficients (Wang, 2000).

Light scattering by a homogeneous sphere coated with a homogeneous layer of uniform thickness was first solved by Aden and Kerker (1951), followed by improvements such as the computation code contributed by Bohren and Huffman (1983), which, however introduced certain computational difficulties in practical applications. For better numerical accuracy, Toon and Ackerman (1981) suggested a more efficient and numerically stable algorithm, though the speed is not very high for large spheres. This paper proposes an efficient, fast, numerically stable and accurate calculation method.

2. Theoretical background

According to the classical Mie theory, physical quantities of the coated sphere such as extinction efficiency k_{ext} , scattering efficiency k_{sca} , absorbing efficiency k_{abs} , the complex scattering amplitudes for two orthogonal directions of incident polarization s_1 and s_2 , as well as the scattering intensities i_1 and i_2 are expressed as (Kerker, 1969; Van de Hulst, 1957):

$$k_{\text{ext}} = \frac{2}{\alpha_1^2} \sum_{n=1}^{\infty} (2n+1) \operatorname{Re}(a_n + b_n),$$
 (1)

$$k_{\text{sca}} = \frac{2}{\alpha_1^2} \sum_{n=1}^{\infty} (2n+1)(|a_n|^2 + |b_n|^2), \tag{2}$$

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(3)

(20)

$$k_{\rm abs} = k_{\rm ext} - k_{\rm sca},$$

$$s_1 = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} (a_n \pi_n + b_n \tau_n), \tag{4}$$

$$s_2 = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} (a_n \tau_n + b_n \pi_n), \tag{5}$$

$$i_1 = |s_1|^2$$
, (6) with the initial values as

$$i_2 = |s_2|^2,$$
 (7) $\psi_0(z) = \sin z,$

 $\chi_0(z) = \cos z$

Bohren and Huffman (1983) expressed the original equations for Mie scattering coefficients a_n and b_n as

$$a_{n} = \frac{\psi_{n}(\alpha_{1}) \left[\psi'_{n}(m_{1}\alpha_{1}) - A_{n} \chi'_{n}(m_{1}\alpha_{1}) \right] - m_{1} \psi'_{n}(\alpha_{1}) [\psi_{n}(m_{1}\alpha_{1}) - A_{n} \chi_{n}(m_{1}\alpha_{1})]}{\zeta_{n}(\alpha_{1}) [\psi'_{n}(m_{1}\alpha_{1}) - A_{n} \chi'_{n}(m_{1}\alpha_{1})] - m_{1} \zeta'_{n}(\alpha_{1}) [\psi_{n}(m_{1}\alpha_{1}) - A_{n} \chi_{n}(m_{1}\alpha_{1})]},$$
(8)

$$b_n = \frac{m_1 \psi_n(\alpha_1) [\psi'_n(m_1 \alpha_1) - B_n \chi'_n(m_1 \alpha_1)] - \psi'_n(\alpha_1) [\psi_n(m_1 \alpha_1) - B_n \chi_n(m_1 \alpha_1)]}{m_1 \zeta_n(\alpha_1) [\psi'_n(m_1 \alpha_1) - B_n \chi'_n(m_1 \alpha_1)] - \zeta'_n(\alpha_1) [\psi_n(m_1 \alpha_1) - B_n \chi_n(m_1 \alpha_1)]},$$
(9)

$$A_n = \frac{m_1 \psi_n(m_1 \alpha_2) \psi_n'(m_2 \alpha_2) - m_2 \psi_n'(m_1 \alpha_2) \psi_n(m_2 \alpha_2)}{m_1 \chi_n(m_1 \alpha_2) \psi_n'(m_2 \alpha_2) - m_2 \chi_n'(m_1 \alpha_2) \psi_n(m_2 \alpha_2)}, \quad (10)$$

$$B_{n} = \frac{m_{1}\psi_{n}(m_{2}\alpha_{2})\psi'_{n}(m_{1}\alpha_{2}) - m_{2}\psi_{n}(m_{1}\alpha_{2})\psi'_{n}(m_{2}\alpha_{2})}{m_{1}\chi'_{n}(m_{1}\alpha_{2})\psi_{n}(m_{2}\alpha_{2}) - m_{2}\psi'_{n}(m_{2}\alpha_{2})\chi_{n}(m_{1}\alpha_{2})},$$
(11)

where m_1 and m_2 are the complex refractive indices of the shell and core relative to the surrounding medium; $\alpha_1 = \pi x_1/\lambda$, $\alpha_2 = \pi x_2/\lambda$ are the corresponding size parameters, in which x_1 and x_2 are outer and inner diameters of the sphere and λ is the wavelength of the incident light in the surrounding free space; and $\psi_n(z)$, $\chi_n(z)$ and $\zeta_n(z)$ are Riccati-Bessel functions of complex argument z, which can be expressed as

$$\psi_n(z) = \sqrt{\frac{\pi z}{2}} J_{n+(1/2)}(z),$$
(12)

$$\chi_n(z) = -\sqrt{\frac{\pi z}{2}} N_{n+(1/2)}(z), \tag{13}$$

$$\zeta_n(z) = \sqrt{\frac{\pi z}{2}} H_{n+(1/2)}^{(2)}(z), \tag{14}$$

where $J_{n+(1/2)}(z)$, $N_{n+(1/2)}(z)$ represent, respectively, the halfinteger-order Bessel functions of the first and second kind, and $H_{n+(1/2)}^{(2)}(z)$ represents the half-integer-order Hankel function of the second kind. These functions satisfy the relations

$$H_{n+(1/2)}^{(2)}(z) = J_{n+(1/2)}(z) - iN_{n+(1/2)}(z), \tag{15}$$

$$\zeta_n(z) = \psi_n(z) + i\chi_n(z). \tag{16}$$

It is very important to point out that the Hankel function of the second kind is chosen to express $\zeta_n(z)$ and hence the imaginary parts of the refractive indices of the shell and the core are negative. However, some researchers tend to use the Hankel function of the first kind so that the imaginary parts of the refractive indices would be positive.

functions $\psi_n(z)$, $\chi_n(z)$ and $\zeta_n(z)$. And $F_n(z)$ satisfies the general recursion relations (Shen & Liu, 2005):

Now $F_n(z)$ is use to represent an arbitrary function of the

$$F_n(z) = \frac{2n-1}{z} F_{n-1}(z) - F_{n-2}(z), \tag{17}$$

$$F'_n(z) = F_{n-1}(z) - \frac{n}{z} F_n(z), \tag{18}$$

$$A = A \times (m_1\alpha_1)$$

$$\zeta_0(z) = \sin z + i\cos z,\tag{21}$$

$$\psi_0'(z) = \cos z,\tag{22}$$

$$\chi_0'(z) = \sin z \tag{23}$$

$$\zeta_0'(z) = \cos z - i\sin z. \tag{24}$$

Although Eqs. (1)–(7) appear to be straightforward, it may lead to failure when one directly uses Bohren and Huffman's codes (1983). The reason for this is that the difference of the terms in Eqs. (10) and (11) in certain order is so small that the digit accuracy decreases, which leads to large errors in the recurrence. In addition, when the complex argument is large, the magnitude of a Bessel function increases exponentially and may exceed the limits of the computer (Yang, 2003). Therefore it is essential to propose an improved algorithm which is more efficient, accurate, fast and numerically stable.

3. Improved computation scheme

We rely on the recursive method and quote the functions that are modified to avoid the computational difficulties. These functions are related with the Riccati-Bessel functions and can be calculated by corresponding recurrence algorithm.

3.1. Complex function $L_n(z)$

A complex function $L_n(z)$ is introduced with the ratio of the Riccati-Bessel functions:

$$L_n(z) = \frac{\psi_n'(z)}{\psi_n(z)}. (25)$$

The numerical results indicate that it is stable and accurate to calculate the function $L_n(z)$ with downward recurrence when the argument z is real or complex (Bayvel & Jones, 1981; Dave, 1968,1969,1970; Du, 2004; Kattawar & Plass, 1967; Shen &

Liu, 2005; Yang, 2003). The downward recurrence is expressed

$$L_{n-1}(z) = \frac{n}{z} - \frac{1}{(n/z) + L_n(z)},$$
(26)

and the initial value $L_{n^*}(z)$ of the downward recurrence can be worked out by the Lentz's method (Lentz, 1976), in which the starting order n^* is to be described in the following part.

3.2. Complex function $N_n(z)$

We introduce a complex function $N_n(z)$, defined as

$$N_n(z) = \frac{\zeta_n'(z)}{\zeta_n(z)}. (27)$$

Although the recurrence relation of $N_n(z)$ is the same as $L_n(z)$, their initial values are different. For this reason the calculation of $N_n(z)$ leads to failure by the downward recurrence with the initial value sought by Lentz's method (Lentz, 1976). Fortunately, the calculation results of the function $N_n(z)$ indicate that it is stable and accurate when the upward recurrence is executed with the argument z being real or complex (Mackowski, Altenkirch, & Menguc, 1990). The upward recurrence is expressed as

$$N_n(z) = -\frac{n}{z} + \frac{1}{(n/z) - N_{n-1}(z)}. (28)$$

beginning with $N_0(z) = -\mathrm{i}$ (when the imaginary part of the refractive index of the sphere is negative). In addition, $N_n(z) \approx -L_n(z)$ as the order n is very large.

3.3. Complex function $M_n(z)$

The complex function $M_n(z)$ is defined as

$$M_n(z) = \frac{\psi_n(z)}{\zeta_n(z)}. (29)$$

Then we can get the recurrence relation of $M_n(z)$ using the calculated $L_n(z)$ and $N_n(z)$ defined above. And $M_n(z)$ can be expressed with the upward recurrence as

$$M_n(z) = M_{n-1}(z) \frac{L_{n-1}(z) - n/z}{N_{n-1}(z) - n/z},$$
(30)

beginning with $M_0(z) = \sin z/(\sin z + i\cos z)$. When the argument z is real, $|M_n(z)|$ is found to be bounded and $|M_n(z)| \le 1$. When the order n is large enough (n > z), $|M_n(z)|$ sharply decreases as n increases. However, when the argument z is complex, $|M_n(z)|$ becomes very large along with the increase of the imaginary part of z, even leading to the overflow failure (see Fig. 1).

3.4. Complex function $Q_n(z_1, z_2)$

Finally we introduce a complex function $Q_n(z_1, z_2)$ expressed as

$$Q_n(z_1, z_2) = \frac{M_n(z_2)}{M_n(z_1)},\tag{31}$$

the recurrence relation of which, after substitution, is given by

$$Q_n(z_1, z_2) = Q_{n-1}(z_1, z_2) \frac{[L_n(z_1) + (n/z_1)][N_n(z_2) + (n/z_2)]}{[L_n(z_2) + (n/z_2)][N_n(z_1) + (n/z_1)]},$$
(32)

beginning with $Q_0(z_1, z_2) = (1 + \text{icot}(z_1))/(1 + \text{icot}(z_2))$. While $|z_1| > |z_2|$ and z_1 and z_2 are real or complex, the recurrence relation expressed in Eq. (32) is stable and $Q_n(z_1, z_2)$ converges with

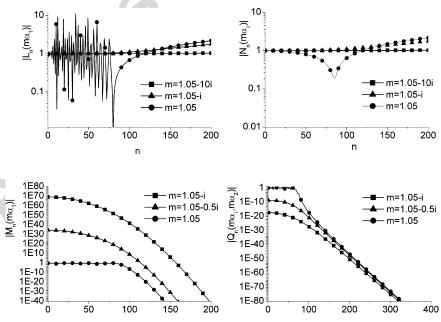


Fig. 1. Results of $|L_n|$, $|N_n|$, $|M_n|$ and $|Q_n|$ with real or complex arguments for $\alpha_1 = 80$ and $\alpha_2 = 60$.

the increase of order n (Yang, 2003). Actually, through the recast of the original equations for Mie scattering coefficients (see Eqs. (33) and (34)), we can see that the introduction of $Q_n(z_1, z_2)$ can overcome the overflow of $M_n(z)$ when the argument is complex, as was discussed in the above section. As an example of this, the calculated numerical values of $|L_n(m\alpha_1)|$, $|N_n(m\alpha_1)|$, $|M_n(m\alpha_1)|$ and $|Q_n(m\alpha_1, m\alpha_2)|$ for $\alpha_1 = 80$ and $\alpha_2 = 60$ are plotted in Fig. 1.

Thereafter all the introduced functions are taken into Eqs. (8)–(11), and we educe

$$a_n = M_n(\alpha_1)C_n(m_1, m_2, \alpha_1, \alpha_2),$$
 (33)

$$b_n = M_n(\alpha_1) D_n(m_1, m_2, \alpha_1, \alpha_2),$$
 (34)

in which $C_n(m_1, m_2, \alpha_1, \alpha_2)$ and $D_n(m_1, m_2, \alpha_1, \alpha_2)$ are defined

In light of Eqs. (33) and (34) and the analysis of Fig. 2, we can see the stopping order n^c is determined by $M_n(\alpha_1)$. Therefore, the property of $M_n(z)$ with a real argument as discussed in Part 3 can be used to determine the stopping order n^c :

$$n^{c} = \begin{cases} \alpha_{1} + 7.5\alpha_{1}^{0.34} + 2, & |M_{n}(\alpha_{1})| < 10^{-18} \\ \alpha_{1} + 6\alpha_{1}^{1/3} + 2, & |M_{n}(\alpha_{1})| < 10^{-12} \\ \alpha_{1} + 4\alpha_{1}^{1/3} + 1, & |M_{n}(\alpha_{1})| < 10^{-6} \\ \alpha_{1} + 4.88\alpha_{1}^{0.31}, & |M_{n}(\alpha_{1})| < 10^{-5} \end{cases}$$
(37)

Eq. (37) shows that we can choose the different stopping order n^c according to the variant precision and it differs from the criterion given by Wiscombe (1980).

In the discussion of the starting order n^* in the downward recurrence of $L_n(z)$, some authors suggested that the downward

$$C_{n}(m_{1}, m_{2}, \alpha_{1}, \alpha_{2}) = \frac{[L_{n}(m_{1}\alpha_{1}) - m_{1}L_{n}(\alpha_{1})] + Q_{n}(m_{1}\alpha_{1}, m_{1}\alpha_{2})(m_{1}L_{n}(m_{2}\alpha_{2}) - m_{2}L_{n}(m_{1}\alpha_{2}))/}{[L_{n}(m_{1}\alpha_{1}) - m_{1}N_{n}(\alpha_{1})] + Q_{n}(m_{1}\alpha_{1}, m_{1}\alpha_{2})(m_{1}L_{n}(m_{2}\alpha_{2}) - m_{2}L_{n}(m_{1}\alpha_{2}))/},$$

$$(35)$$

$$(m_{1}L_{n}(m_{2}\alpha_{2}) - m_{2}N_{n}(m_{1}\alpha_{2}))[m_{1}N_{n}(\alpha_{1}) - N_{n}(m_{1}\alpha_{1})]$$

$$D_{n}(m_{1}, m_{2}, \alpha_{1}, \alpha_{2}) = \frac{\left[m_{1}L_{n}(m_{1}\alpha_{1}) - L_{n}(\alpha_{1})\right] + Q_{n}(m_{1}\alpha_{1}, m_{1}\alpha_{2})(m_{2}L_{n}(m_{2}\alpha_{2}) - m_{1}L_{n}(m_{1}\alpha_{2}))/}{\left[m_{2}L_{n}(m_{2}\alpha_{2}) - m_{1}N_{n}(m_{1}\alpha_{2})\right]\left[L_{n}(\alpha_{1}) - m_{1}N_{n}(m_{1}\alpha_{1})\right]} - \frac{\left(m_{2}L_{n}(m_{2}\alpha_{2}) - m_{1}N_{n}(m_{1}\alpha_{2})\right)\left[L_{n}(\alpha_{1}) - m_{1}N_{n}(m_{1}\alpha_{2}) - m_{1}L_{n}(m_{1}\alpha_{2})\right)/}{\left[m_{2}L_{n}(m_{2}\alpha_{2}) - m_{1}N_{n}(m_{1}\alpha_{2})\right)\left[N_{n}(\alpha_{1}) - m_{1}N_{n}(m_{1}\alpha_{1})\right]}$$
(36)

The numerical results of $|C_n(m_1, m_2, \alpha_1, \alpha_2)|$ and $|D_n(m_1, m_2, \alpha_1, \alpha_2)|$ for $\alpha_1 = 80$ and $\alpha_2 = 60$ are plotted in Fig. 2. Four cases are tested, respectively: an absorbent core and a transparent shell; a transparent core and a transparent core and a transparent shell; an absorbent core and an absorbent shell. Fig. 2 shows that, in all cases, $|C_n(m_1, m_2, \alpha_1, \alpha_2)|$ and $|D_n(m_1, m_2, \alpha_1, \alpha_2)|$ oscillate violently for small orders n and then decrease along with the increase of the order n.

recursion should start with $\psi_{n^*}(z) = 0 + i0$ and $\psi_{n-1^*}(z) = 1 + i0$ (or $L_{n^*}(z) = 0 + i0$), whereby the order n^* would be large enough to make the recurrence converge at the cutoff order n^c , which was determined by the Kapteyn inequality (Watson, 1966). Some other authors, such as Wang and van de Hulst (1991), used the asymptotic value as the starting value. Kattawar and Plass (1967) proved that the computational error decreased

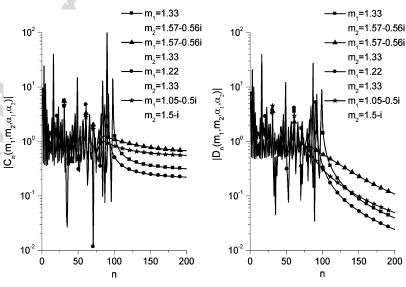


Fig. 2. Results of $|C_n(m_1, m_2, \alpha_1, \alpha_2)|$ and $|D_n(m_1, m_2, \alpha_1, \alpha_2)|$ with real or complex arguments for $\alpha_1 = 80$ and $\alpha_2 = 60$.

at each step if $L_n(z)$ was calculated by downward recurrence and the calculation started at some value $n^* \gg |z|$. An example of this is the work presented by Du (2004). Therefore through numerous recurrences, the calculation of above methods can then converge to the correct value. That is to say, the recurrence times have to be extremely large when the argument z is very large. The disadvantage of this is that we have to calculate the functions $L_{n^*}(\alpha_1)$, $L_{n^*}(m_1\alpha_1)$, $L_{n^*}(m_1\alpha_2)$ and $L_{n^*}(m_2\alpha_2)$, starting from $n^* \gg |\alpha_1|, n^* \gg |m_1\alpha_1|, n^* \gg |m_1\alpha_2|$ and $n^* \gg |m_2\alpha_2|$, respectively. So, if the refractive indices are very large, values of these functions of the high orders (i.e. those for $n^* > n^c$) have to be calculated, which however will never be used in further calculation of the scattering quantities. This makes the calculation extremely expensive. Another disadvantage of the determination of the starting order n^* in the downward recurrence of $L_n(z)$ proposed by the earlier authors may also occur, when the relative refractive indices are smaller than 1. It was mentioned above that the calculation of the function $L_n(z)$ starts from an order $n^* \gg |z|$, as determined with the criterion proposed by Wiscombe (1980). Unfortunately, this only insures that all the necessary orders of $L_n(\alpha_1)$ are calculated. While the refractive indices are smaller than 1, the starting order n^* for the calculation of $L_n(m_1\alpha_1)$, $L_n(m_1\alpha_2)$ or $L_n(m_2\alpha_2)$ is possibly smaller than the stopping order n^c , which might lead to the lack of some necessary values of these functions for the further calculation of the Mie scattering coefficients a_n and b_n , and thus result in failure.

However, the stopping order n^c can be chosen according to Eq. (37) and the value of the function $L_{n^c}(z)$ can be calculated directly with the Lentz's method (Lentz, 1976), without many recurrences that demand $n^* \gg n^c$. In this way, both of the disadvantages discussed above can be avoided.

In conclusion, Mie scattering coefficients a_n and b_n can be successfully computed by Eqs. (33), (34) and (37) while the introduced functions $L_n(z)$, $N_n(z)$, $M_n(z)$, $Q_n(z_1, z_2)$ and the stopping order n^c of the downward recurrence are worked out. By the proper recurrence relations we can calculate the Mie scattering coefficients of a coated sphere with arbitrary parameters (i.e. shell and core diameters, and refractive indices).

Two special cases of light scattering by a coated sphere are discussed in the following text. Setting the refractive indices of the core and coating equal to each other, namely, $m_1 = m_2$, Eqs.

(33) and (34) can be simplified into

$$a_n = M_n(\alpha_1) \frac{L_n(m_1 \alpha_1) - m_1 L_n(\alpha_1)}{L_n(m_1 \alpha_1) - m_1 N_n(\alpha_1)},$$
(38)

$$b_n = M_n(\alpha_1) \frac{m_1 L_n(m_1 \alpha_1) - L_n(\alpha_1)}{m_1 L_n(m_1 \alpha_1) - N_n(\alpha_1)}.$$
(39)

In this way a_n and b_n become the Mie scattering coefficients of a homogeneous sphere with the refractive index m_1 and the size parameter α_1 (Shen & Liu, 2005).

Another special case is that while the refractive index of coating $m_1 = 1$, Mie coefficients can be simplified into

$$a_n = M_n(\alpha_2) \frac{L_n(m_2\alpha_2) - m_2 L_n(\alpha_2)}{L_n(m_2\alpha_2) - m_2 N_n(\alpha_2)},$$
(40)

$$b_n = M_n(\alpha_2) \frac{m_2 L_n(m_2 \alpha_2) - L_n(\alpha_2)}{m_2 L_n(m_2 \alpha_2) - N_n(\alpha_2)}.$$
(41)

In this way a_n and b_n become the Mie scattering coefficients of a homogeneous sphere with the refractive index m_2 and the size parameter α_2 . Correspondingly, the particle size parameter α_1 in Eqs. (1) and (2) must be replaced with α_2 .

4. Results and discussion

Exemplifying results are obtained with a double-precision VC++6.0 code on a personal computer powered by a 2.4 GHz P4 CPU.

As an example of strongly absorbent spheres, the results of $L_n(m\alpha)$ with $\alpha=80$ and m=1.05-i are given in Table 1, comparing with those by Yang (2003) and those by Lentz (1976). For adopting the positive imaginary part of the refractive index, the calculated imaginary part of $L_n(z)$ by Yang is negative but it is positive as calculated by Lentz and with our method. When the order n is small, values of $L_n(z)$ of the three methods match comparatively. However, when n becomes large, the values of $L_n(z)$ by Yang differ greatly from those by Lentz's method and ours. This is because Yang chose a value of starting order n^* for the downward recurrence different from ours. Lentz's method was proved to be correct previously (Bayvel & Jones, 1981); so apparently, our method is more accurate than Yang's.

Cases are tested on the condition of the refractive indices of the coating $m_1 = 1.33$ and the core $m_2 = 1.59 - 0.66$ i, the core size parameter $\alpha_2 = 0.5$ and different values of the coating size parameter α_1 . Only the computational time, extinction efficiency

Table 1 Comparison of $L_n(z)$ calculated by Yang, Lentz and this study

n	$L_n(z)$					
	Yang (2003)	Lentz (1976)	This work			
0	(0.11449E-15, -0.10000E+01)	(1.05818E-16, 1.00000)	(1.05818E-16, 1.00000)			
1	(0.74646E-04, -0.10000E+01)	(7.46460E-05, 9.99996E-01)	(7.46460E-05, 9.99996E-01)			
30	(0.34764E-01, -0.99870)	(3.47638E-02, 9.98696E-01)	(3.47638E-02, 9.98696E-01)			
60	(0.13645, -0.10019E+01)	(1.36451E-01, 1.00190)	(1.36451E-01, 1.00190)			
90	(0.29777, -0.10278E+01)	(2.97771E-01, 1.02775)	(2.97771E-01, 1.02775)			
116	(0.46923, -0.10806E+01)	(0.46923, 1.080629)	(0.46923, 1.080629)			
130	(0.17656, -0.13895E+01)	(5.67383E-01, 1.12111)	(5.67383E-01, 1.12111)			

Table 2 Comparison of CPU time, $k_{\rm ext}$ and $k_{\rm sca}$ calculated by T–A and this study

α_1	CPU time (s)		$k_{ m ext}$		$k_{ m sca}$	
	T–A	This study	T–A	This study	T–A	This study
1	9.46E-05	1.16E-04	0.366043	0.366043	0.124027	0.124027
10	2.00E-04	2.67E - 04	2.210291	2.210291	2.206762	2.206762
40	5.18E-04	6.34E - 04	1.987762	1.987762	1.987576	1.987576
70	9.64E-04	9.93E-04	2.021424	2.021424	2.021344	2.021344
100	1.39E-03	1.30E-03	2.101052	2.101052	2.101013	2.101013
500	6.24E-03	5.11E-03	2.030372	2.030372	2.030371	2.030371
1000	1.20E-02	9.76E - 03	2.016579	2.016579	2.016578	2.016578
5000	5.70E-02	4.50E-02	2.005736	2.005736	2.005736	2.005736

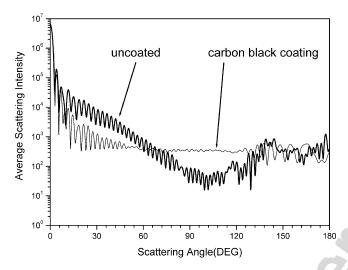


Fig. 3. Average scattering intensity as a function of scattering angle for a homogeneous (uncoated) water sphere and a composite water–carbon sphere. In both cases the whole particle $\alpha_1 = 70$; the coated sphere shell thickness is 1%, the refractive index of water $m_2 = 1.33 - i0$, the refractive index of the carbon coating $m_1 = 2 - i1$.

 $k_{\rm ext}$ and absorbing efficiency $k_{\rm abs}$ are compared. As an example of this, results on $k_{\rm ext}$ and $k_{\rm sca}$ are given in Table 2, comparing with those given by Toon and Ackerman (1981), denoted as T–A. Table 2 shows that the calculation speed of our method is a little slower than that of the T–A algorithm if $\alpha_1 < 100$. However, if $\alpha_1 \ge 100$, our method works faster than the T–A algorithm. Accordingly, our method is more suitable for calculating large coated spheres. In addition, the results of $k_{\rm ext}$ and $k_{\rm sca}$ with the two algorithms have perfect match.

In Fig. 3 the average scattering intensity $(i_1/i_2)/2$ is plotted versus the scattering angle for a water droplet with a whole particle size parameter $\alpha_1 = 70$, and a 1%-thick coating of carbon (core $m_2 = 1.33 - i0$ (water) and shell $m_1 = 2 - i1$). As shown, the present equations yield results in good agreement with the results given by Miroslaw (2006) who employs the T-A algorithm.

5. Conclusions

An improved and more efficient algorithm to calculate Mie scattering coefficients a_n and b_n for a coated sphere is presented, using complex functions $L_n(z)$, $N_n(z)$, $M_n(z)$ and $Q_n(z_1, z_2)$ to

recast the coefficients. And we also test the convergent property of the fractions $|C_n(m_1, m_2, \alpha_1, \alpha_2)|$ and $|D_n(m_1, m_2, \alpha_1, \alpha_2)|$ in the expression of a_n and b_n . $M_n(\alpha_1)$ can be used to determine the stopping order n^c of the summation of the Mie scattering coefficients a_n and b_n that can be chosen differently according to the variant precision of the calculation. The starting order n^* of the function $L_n(z)$ is equal to n^c .

As a result, this algorithm overcomes the numerical difficulties. Exemplifying results are given to check the accuracy, stability and reliability of our method for a large range of size parameter and refractive index. And the results show good agreement with other published results. In addition, our method is much simpler and the calculation speed is much fast for large particles.

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References

Aden, A. L., & Kerker, M. (1951). Scattering of electromagnetic waves from two concentric spheres. *Journal of Applied Physics*, 22(10), 1242–1246.

Bayvel, L.P., & Jones, A.R. (1981). *Electromagnetic scattering and its applications* (pp. 26–27). London: Applied Science.

Bohren, C. F., & Huffman, D. R. (1983). *Absorption and scattering of light by small particles*. New York: John Wiley & Sons.

Choi, M. K. (2001). Numerical calculation of light scattering from a layered sphere by the boundary-element method. *Journal of the Optical Society of America A*, 18(3), 577–583.

Dave, J.V. (1968). Subroutines for computing the parameters of the electromagnetic radiation scattering by spheres. Report No. 320-3237, IBM Scientific Center, Palo Alto, CA.

Dave, J. V. (1969). Scattering of electromagnetic radiation by a large, absorbing sphere. IBM Journal of Research and Development, 13, 302–313.

Dave, J. V. (1970). Coefficients of the Legendre and Fourier series for the scattering functions of spherical particles. *Applied Optics*, 9(8), 1888–1896.
 Du, H. (2004). Mie-scattering calculation. *Applied Optics*, 43(9), 1951–1956.

He, W. D., & Pan, C. Y. (1997). Core-shell polymer particles. *Journal of Functional Polymer*, 10(1), 110–117 (in Chinese).

Kattawar, G. W., & Plass, G. N. (1967). Electromagnetic scattering from absorbing sphere. Applied Optics, 6(8), 1377–1382.

Kerker, M. (1969). The scattering of light and other electromagnetic radiation. New York: Academic Press.

- Lentz, W. J. (1976). Generating Bessel functions in Mie scattering calculations using continued fractions. *Applied Optics*, *15*(3), 668–671.
- Mackowski, D. W., Altenkirch, R. A., & Menguc, M. P. (1990). Internal absorption cross sections in a stratified sphere. *Applied Optics*, 29(10), 1551–1559.
- Miroslaw, J. (2006). Light scattering calculator: Coated sphere. Retrieved September 30, 2004, from http://www.mjcopticaltech.com/Products/ LscCoatSphHelp.htm.
- Shen, J., & Liu, L. (2005). An improved algorithm of classical Mie scattering calculation. *China Powder Science and Technology*, 11(4), 1–5 (in Chinese)
- Toon, O. B., & Ackerman, T. P. (1981). Algorithms for the calculation of scattering by stratified spheres. *Applied Optics*, 20(20), 3657–3660.
- Van de Hulst, H. C. (1957). Light scattering by small particles. New York: Wiley. Wang, N. N. (Ed.). (2000). Optical measurement and application of particle size. Beijing: Atomic Energy Press (in Chinese).
- Wang, R. T., & van de Hulst, H. C. (1991). Rainbows: Mie computations and the airy approximation. *Applied Optics*, 30(1), 106–117.
- Watson, G. N. (1966). A treatise on the theory of Bessel functions. London: Cambridge U. Press.
- Wiscombe, W. J. (1980). Improved Mie scattering algorithms. Applied Optics, 19(9), 1505–1509.
- Yang, W. (2003). Improved recursive algorithm for light scattering by a multilayered sphere. Applied Optics, 42(9), 1710–1720.