International Journal of Theoretical Physics, Vol. 36, No. 4, 1997

Radiative Transfer Single-Scattering Albedo Estimation with a Super-Padé Approximation of Chandrasekhar's *H*-Function

Eric Steinfelds,[1] Mark A. Samuel,[1] N. J. McCormick,[2] and James H. Reid[3]

Received October 16, 1996

Three algorithms for evaluating the single-scattering albedo within an isotropically scattering, semi-infinite medium are developed for measurements external to the medium with narrow and wide field-of-view detectors. Two of the algorithms are iterative and require the computation of the Chandrasekhar H-function, which can be done with the super-Padé approximation, while the third algorithm is an explicit one that requires no iteration.

1. INTRODUCTION

The objective of this work is twofold: (a) to formulate the solution of an inverse radiative transfer problem for estimating the single-scattering albedo ϖ of a large (effectively semi-infinite) isotropic scattering medium that is illuminated uniformly over its surface, and (b) to introduce another way of approximately evaluating the Chandrasekhar (1960) H-function that can be used in the solution of the inverse problem.

Depending on the detector(s) available and the direction(s) of the source illuminating the surface, different algorithms are needed to solve the inverse problem for ϖ. For an azimuthally symmetric, multidirectional incident illumination, Siewert (1978) developed a succinct set of equations for determining ϖ from angular moments of the outgoing radiance measured over all polar angles. But to minimize the need for a multidirectional source and to reduce

[1]Department of Physics, Oklahoma State University, Stillwater, Oklahoma 74078.
[2]Department of Mechanical Engineering, University of Washington, Seattle, Washington 98195-2600.
[3]L. H. Lanzl Institute of Medical Physics, Seattle, Washington 98119.

0020-7748/97/0400-0997$12.50/0

the number of measurement directions, we will assume a normally incident illumination, as is typical of many laboratory-scale experiments done with a beam-expanded laser illuminating a flat surface of a target. If the H-function is computed, only two measurements then are needed, the inward and outward fluxes [as measured with a flat-surface hemispherical (2π) field-of-view (FOV) detector] or the normally-directed inward and outward radiances (as measured with a narrow FOV detector). If the outward flux and normally directed outward radiance are measured along with the inward flux or normally direct inward radiance (which should be identical), then the two algorithms involving the H-function can be combined in such a way that no H-function computations or iterations are required in an explicit algorithm. The two iterative algorithms apparently are new, while the explicit algorithm is a special case of one derived by Siewert (1979).

The choice of which algorithm to use is thus dictated by the detectors available. If only a flux or radiance detector is available, then one of the two iterative algorithms obtained here may be useful, provided the H-function can be readily computed. Several approximate methods have been used to evaluate the H-function (Abu-Shumays, 1966, 1967; Kelley, 1978, 1980, 1982), including a low-level Padé approximation (Abu-Shumays, 1967). Typically such approximations are computationally more rapid than highly accurate methods, such as that developed by Dunn *et al.* (1982).

A super-Padé approximation technique is explored here as a possible computational technique for the H-function. This numerical approximation method relies on the use of Padé approximants to solve the nonlinear integral equation

$$H(z) = 1 + \frac{\varpi z}{2} H(z) \int_0^1 \frac{H(\mu)}{z + \mu}\, d\mu, \qquad z \notin [-1, 0] \tag{1}$$

where ϖ is the single-scattering albedo and z is a complex variable. An important constraint on $H(z)$ is that $H^{-1}(-\nu_0) = 0$, where $\nu_0 > 1$ is the positive discrete eigenvalue of the homogeneous radiative transport equation, as given by the positive root of

$$\frac{\varpi z}{2} \ln\left[\frac{z+1}{z-1}\right] = 1, \qquad z \notin [-1, 1] \tag{2}$$

In the method of Padé approximants (Baker, 1975; Bender and Orszag, 1978) a function is approximated by a ratio of two polynomials. For a given power series

$$S(z) = S_0(z) + S_1(z)\varpi + \cdots + S_J(z)\varpi^J \tag{3}$$

where $J = N + M$, a Padé approximant (PA) is written as

$$[N/M] = \frac{a_0(z) + a_1(z)\varpi + \cdots + a_N(z)\varpi^N}{1 + b_1(z)\varpi + \cdots + b_M(z)\varpi^M} \tag{4}$$

where $[N/M] = S(z) + O(\varpi^{J+1})$. Once the coefficients $a_i(z)$ and $b_i(z)$ have been determined, a Padé approximant prediction (PAP) for the next coefficient in the power series $S_{J+1}(z)$ follows from the PA. Also, an estimate of the sum of the series, i.e., the full Padé summation (FPS), can be obtained. The PAP and FPS have been applied with remarkable success to the perturbation expansions of quantum field theory and statistical mechanics by Samuel *et al.* (1995a,b) and (Ellis *et al.*, 1996).

The method of PA can be used to accelerate the convergence of iterative solutions of Fredholm-type integral equations. The nonlinear integral equation for the H-function in (1) is of a type to which this method can be applied. In this instance, the power series expansion is taken in terms of the albedo ϖ.

Siewert's (1978, 1979) algorithms and the two algorithms that require the H-function for solving the inverse problem are given in Section 2. Section 3 contains a detailed exposition of the numerical algorithms used to evaluate the H-function with super-Padé approximations and Section 4 provides some numerical results for the H-function approximations.

2. INVERSE ALBEDO ESTIMATION ALGORITHMS

The radiation intensity $I(x, \mu)$ for $x \geq 0$ is taken to be a function of the direction cosine μ measured with respect to the (dimensionless) mean-free-path distance x from the surface into the semi-infinite medium. For isotropic scattering the radiative transfer equation for the semi-infinite medium is

$$\mu \frac{\partial}{\partial x} I(x, \mu) + I(x, \mu) = \frac{\varpi}{2} \int_{-1}^{1} I(x, \mu')\, d\mu', \qquad x > 0 \tag{5}$$

for $\varpi < 1$, where

$$I(x, \mu) = \int_0^{2\pi} I(x, \mu, \phi)\, d\phi \tag{6}$$

and ϕ is the azimuthal angle measured in the plane perpendicular to the x axis. The half-space problem is defined by the incident illumination

$$I(0, \mu) = F(\mu), \qquad \mu > 0 \tag{7}$$

and the constraint that $I(x, \mu) \to 0$ as $x \to \infty$. Chandrasekhar (1960) has shown that the radiation emerging from the half-space is given by

$$I(0, -\mu) = \frac{\varpi}{2} H(\mu) \int_0^1 \frac{H(\mu')F(\mu')\mu'}{\mu' + \mu} d\mu', \qquad \mu > 0 \tag{8}$$

where $H(\mu)$ satisfies equation (1).

Siewert (1978) showed for the general class of "β" boundary conditions defined by $F(\mu) = K\mu^\beta$, $\mu > 0$, that if various angular moments of the emerging radiance $I^{(\beta)}(0, -\mu)$ are measured, as defined by

$$E_\alpha^{(\beta)} = \int_0^1 I^{(\beta)}(0, -\mu)\mu^\alpha \, d\mu \tag{9}$$

then ϖ can be estimated from any of the set of equations

$$\varpi = 4 \frac{K^{-1}E_\beta^{(\beta)}}{[K^{-1}E_0^{(\beta)} + (\beta + 1)^{-1}]^2}, \qquad \beta = 0, 1, 2, \ldots \tag{10}$$

Here K is the magnitude of the incoming flux as measured with a 2π FOV detector or the incoming radiance measured with a normally directed, narrow FOV detector.

A major limitation in using this last equation, however, is that the $F(\mu) = K\mu^\beta$ incident illumination is difficult to achieve experimentally and because only the measurement of $E_1^{(\beta)}$ can be conveniently done with a flat-surface hemispherical FOV detector. For this reason we instead force the incident illumination to satisfy the normally incident, "δ"-boundary condition defined by $F(\mu) = K\delta(\mu - 1)$, $\mu > 0$, and observe from equation (8) that the emerging radiance $I^{(\delta)}(0, -\mu)$ is

$$I^{(\delta)}(0, -\mu) = K \frac{\varpi H(1)}{2} \frac{H(\mu)}{\mu + 1}, \qquad \mu > 0 \tag{11}$$

Thus with the use of a normally directed, narrow FOV detector that measures $I^{(\delta)}(0, -1)$,

$$\varpi H^2(1) = 4K^{-1}I^{(\delta)}(0, -1) \tag{12}$$

This is an algorithm for implicitly estimating ϖ using only inward- and outward-directed narrow FOV detector measurements and computation of $\varpi H^2(1)$, which can be easily done with the super-Padé results of Section 3.

Another algorithm that could be conveniently implemented is to use a 2π FOV detector and then measure $E_1^{(\delta)}$, defined similarly to equation (9) with $F(\mu) = K\delta(\mu - 1)$, $\mu > 0$. From equation (11) it then follows that

$$E_1^{(\delta)} = K \frac{\varpi H(1)}{2} \int_0^1 \frac{H(\mu)\mu}{\mu + 1} d\mu \tag{13}$$

But use of a partial fraction expansion and equation (1) shows that

$$\frac{\varpi H(1)}{2}\int_0^1 \frac{H(\mu)\mu}{\mu + 1}\,d\mu = 1 - \left(1 - \frac{\varpi\alpha_0}{2}\right)H(1) \tag{14}$$

where $\alpha_k = \int_0^1 \mu^k H(\mu)\,d\mu$. For isotropic scattering (Chandrasekhar, 1960)

$$1 - \frac{\varpi\alpha_0}{2} = (1 - \varpi)^{1/2} \tag{15}$$

so it follows from the last three equations that a second algorithm for estimating ϖ is

$$(1 - \varpi)H^2(1) = (1 - K^{-1}E_1^{(\delta)})^2 \tag{16}$$

This is an algorithm for implicitly estimating ϖ using only inward- and outward-directed 2π FOV detector measurements and computation of $(1 - \varpi)H^2(1)$.

Finally, from the ratio of equations (12) and (16) it follows that

$$\frac{1 - \varpi}{\varpi} = \frac{(1 - K^{-1}E_1^{(\delta)})^2}{4K^{-1}I^{(\delta)}(0, -1)} \tag{17}$$

This third algorithm, one of Siewert's (1979), is an explicit algorithm that does not require computation of $H(1)$, but both the outward-directed narrow FOV and 2π FOV detector measurements and an inward-directed narrow FOV or 2π FOV detector measurement are needed. The result also can be obtained as a special case, for monodirectional illumination and isotropic scattering of a half-space, from an inverse radiative transfer equation (McCormick, 1979) that is a generalization of that of Siewert (1979, equation (31)).

3. APPROXIMANTS FOR THE *H*-FUNCTION

The PA method has been applied in a variety of disciplines. For quantum electrodynamics and quantum chromodynamics, for example, the perturbation series are divergent and may not even be Borel summable and the coefficients in the power series are believed to diverge strongly like $S_n = n!k^n n^\gamma$, where k and γ are constants that depend on the problem under consideration (Vainshtein and Zakharov, 1994). Yet the PAP works well for QED and QCD and also for series generated in statistical mechanics (Samuel *et al.*, 1995a,b; Ellis *et al.*, 1996). Perhaps the ability of a sufficiently complicated rational function to imitate the analytic structure of some given function accounts for this success. For large enough N and M, zeros and poles of any function can be exactly reproduced, and branch points and essential singularities approximated by a set of poles.

To apply the PA method to equation (1) suggests that we rewrite the equation as

$$H(z) = 1 + \varpi H(z) \int_0^1 G(z, \mu) H(\mu)\, d\mu \tag{18}$$

Here ϖ can be viewed as the power series expansion parameter. Let the nth iterate in the Neumann series solution to this equation be $H_n(z)$ and define

$$S_n(z) = \frac{H_{n+1}(z) - H_n(z)}{\varpi^n} \tag{19}$$

Once the $S_n(z)$ have been computed for $n = 1$ to J we construct the PA of equation (4). Then the PA method predicts the next term $S_{J+1}(z)$. In particular,

$$S_0(z) = 1$$

$$S_1(z) = \int_0^1 G(z, \mu)\, d\mu \tag{20a}$$

$$S_2(z) = \int_0^1 G(z, \mu)\, d\mu \int_0^1 G(z, \mu')\, d\mu' \tag{20b}$$

$$+ \int_0^1 \int_0^1 G(z, \mu) G(\mu, \mu')\, d\mu'\, d\mu \tag{20c}$$

$$S_3(z) = \int_0^1 G(z, \mu)\, d\mu \int_0^1 G(z, \mu')\, d\mu' \int_0^1 G(z, \mu'')\, d\mu'' \tag{20d}$$

$$+ \int_0^1 G(z, \mu'')\, d\mu'' \int_0^1 \int_0^1 G(z, \mu) G(\mu, \mu')\, d\mu'\, d\mu \tag{20e}$$

$$+ \int_0^1 \int_0^1 G(z, \mu) G(\mu, \mu')\, d\mu'\, d\mu \int_0^1 G(z, \mu'')\, d\mu'' \tag{20f}$$

$$+ \int_0^1 G(z, \mu) \int_0^1 G(\mu, \mu')\, d\mu' \int_0^1 G(\mu, \mu'')\, d\mu''\, d\mu \tag{20g}$$

$$+ \int_0^1 G(z, \mu) \int_0^1 G(\mu, \mu') \int_0^1 G(\mu', \mu'')\, d\mu''\, d\mu'\, d\mu \tag{20h}$$

etc. The nesting of the integrals in these terms can be represented by diagrams that resemble uncrossed corrections to a propagator in quantum field theory. Figure 1 illustrates the diagrams for the terms (20a)–(20h).

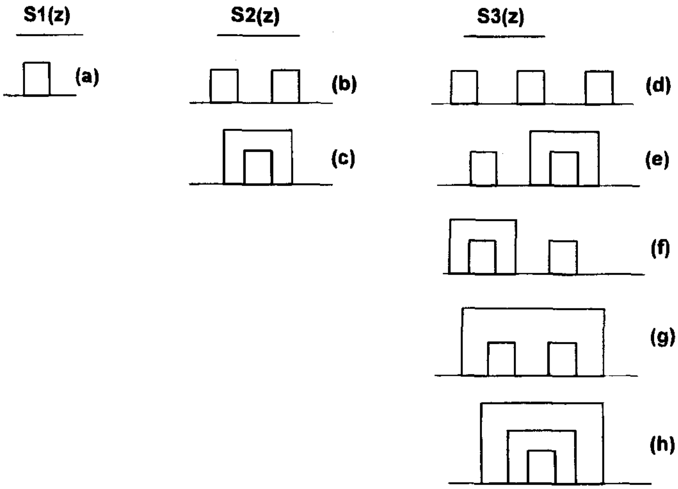

Fig. 1. Diagrams of $S_n(z)$ terms in equation (20) for $n = 1$–3.

Since we have the means to estimate the next term PAP, and we also have error formulas (that include the sign) for the PAP, we can correct the PAP to obtain a more precise estimate that we call the super-Padé approximant prediction (SPAP) defined by

$$\hat{S}_{N+M+1} = \frac{S_{N+M+1}}{1 + r} \tag{21}$$

where S_{N+M+1} is the PAP of equation (3) and $\hat{S}_{N+M+1}$ is the SPAP. For the H-function for $z = 1$, the formula for r for the N/M PAP in equation (21) is (Samuel *et al.*, 1995a; Ellis *et al.*, 1996)

$$r = -M!B(B + 1) \cdots (B + M - 1)/L^{2M} \tag{22}$$

where r is the relative error (i.e., the estimate minus the exact, all divided by the exact) and (Samuel *et al.*, 1995a; Ellis *et al.*, 1996)

$$L = N + M + aM + b \tag{23}$$

In our case the constants B, a, and b were determined by first examining the numerical values of $S_1(1)$ to $S_7(1)$ and comparing the results to those in the following equations (Samuel *et al.*, 1995b):

$$S_{n+2} = S_{n+1}^2/S_n, \qquad [n/1]\text{PAP} \tag{24}$$

$$S_{n+3} = \frac{2S_nS_{n+1}S_{n+2} - S_{n-1}S_{n+2}^2 - S_{n+1}^3}{S_n^2 - S_{n-1}S_{n+1}}, \qquad [n/2]\text{PAP} \tag{25}$$

with $S_j = 0$ for $j < 0$. [Formulas for S_n for $M = 3$ and 4 are also given in Samuel *et al.* (1995b). For general N and M the PAPs are constructed numerically.] We then calculated r for the PAPs for small N and M and determined that r is given by the error formula (22) with $B = 1.34$, $a = -0.5$, and $b = 1.6$. We then used $\hat{S}_{N+M+1}$, applied the PAP again to obtain S_{N+M+2}, and then applied the correction again and after using (21) obtained the SPAP $\hat{S}_{N+M+2}$; the process can be continued indefinitely.

4. NUMERICAL RESULTS FOR THE *H*-FUNCTION

Our results for the number of terms in $S_n(z)$ (i.e., diagrams of Fig. 1) versus n needed for the H-function for $n = 1$ to $n = 11$ are 1, 2, 5, 14, 42, 132, 429, 1430, 4862, 16796, 58786, etc. For the number of terms indicated we checked our predictions by direct counting for $n = 1$ to $n = 9$. The SPAP agrees with the direct counting exactly; in fact, when they initially disagreed for $n = 7$ a check revealed an error in the direct counting. Later a direct calculation of $S_8(1)$ agreed with our estimate to within 0.014%.

In Table I we give the FPS results for the 3/4, 4/3, and the 4/4. The ordinary partial sum (PS) results from equation (3) are also given. It can be seen that in all cases the Padé results are more precise than the corresponding PS results up to $n = 7$. It should be emphasized that the FPS results use the same input as the PS.

Table II contains the coefficients from $n = 0$ to $n = 15$. The results for $n = 0$–5 were used along with the SPAP to obtain the results for $n = 6$ and 7, which agreed with the direct calculation to within <0.1%. The results for $n = 0$–7 were then used to obtain the coefficients for n up to 26 by repeated application of the super-Padé method.

Table I. $H(1)$ Functions Obtained with Padé Approximants and from Partial Sums with Seventh-Order Iterations

ϖ	Pade34	Pade43	Pade44	Partial sum (PS)	"Exact"
0.3	1.1268438	1.1268438	1.126844	1.126843	1.126844
0.5	1.251255	1.251254	1.251257	1.250940	1.251259
0.8	1.597526	1.597457	1.597945	1.571937	1.598219
0.9	1.842901	1.842344	1.846299	1.748239	1.850098
0.95	2.045295	2.043641	2.056968	1.857371	2.077123
0.975	2.189267	2.186171	2.212264	1.918297	2.270984
0.99	2.299123	2.294248	2.334419	1.957090	2.472792
0.995	2.340862	2.335252	2.382079	1.970430	2.587346
1.0	2.385145	2.378988	2.434109	1.983958	2.907809

Table II. Coefficients $S_n(1)$ for $H(1)$ Functions Obtained Directly from Equation (21) up to n = 7 and from the Super-Padé Approximant Prediction for $n \geq 8$

n	$S_n(1)$	n	$S_n(1)$	n	$S_n(1)$
1	0.693147	10	35.257	19	7224.3
2	0.804054	11	62.263	20	13300.4
3	1.096628	12	110.84	21	24549.8
4	1.626989	13	198.62	22	45434.9
5	2.544145	14	357.89	23	84357.1
6	4.125346	15	647.94	24	157341.
7	6.870243	16	1177.9	25	295683.
8	11.6787	17	2149.3	26	563063.
9	20.164	18	3934.6		

Table III gives results for the percent error for the $H(1)$-function when compared with the "exact" results of Stibbs and Weir (1959). The super-Padé evaluation of $H(1)$ is a more severe test of the method than for $H(\mu)$, $0 \leq \mu < 1$, since in general the full Padé summation (FPS) for smaller values of μ are more precise. The FPS is compared with the PS results in Table III for the same number of $S_n(1)$ coefficients, n = 0–7. It can be seen that in all cases the FPS results are much more precise than the PS results.

Table III. $H(1)$ Functions Obtained from the Super-Padé Approximants Prediction (SPAP) and Partial Sum (PS) Methods

ϖ	SPAP/FPS	PS	"Exact"
0.1	1.03682	1.03682	1.036815
0.2	1.07864	1.07861	1.078644
0.3	1.12684	1.12684	1.126844
0.4	1.18337	1.18325	1.183380
0.5	1.25126	1.25094	1.251259
0.6	1.33540	1.33379	1.335406
0.7	1.44469	1.43790	1.444745
0.8	1.59797	1.57195	1.598219
0.85	1.70433	1.65388	1.704991
0.9	1.84833	1.74826	1.850098
0.925	1.94522	1.80082	1.947955
0.95	2.07339	1.85740	2.077123
0.975	2.26728	1.91833	2.270984
0.99	2.46309	1.95713	2.472792
0.995	2.55935	1.97046	2.587346
1.0	2.68543	1.98399	2.907809

5. CONCLUDING COMMENTS

A concise way of estimating the single-scattering albedo ϖ has been developed, along with an approximate method of computing the Chandrasekhar H-function needed for two of the inverse algorithms. Although in this paper we have focused on evaluating algorithms for a normally incident illumination ($\mu = 1$), the algorithms also can be extended to nonnormally incident illumination ($\mu < 1$), but require azimuthally dependent measurements (McCormick, 1979); in such cases, our numerical results for the $H(\mu)$-function, $\mu < 1$, are even better than shown here.

The assumption of isotropic scattering is a severe limitation of the algorithms for many applications, but estimation of ϖ for a general scattering law with narrow FOV measurements over only the azimuthal angle would be difficult to implement because the algorithms become exceedingly complex (Sanchez and McCormick, 1981).

We believe that the super-Padé methods used here may be of practical utility in solving linear integral equations as well as other nonlinear integral equations.

ACKNOWLEDGMENTS

This work was supported in part by the U.S. Department of Energy under grant DE-FG05-84ER40215. The authors appreciate the initiative of David Jette and the Lanzl Institute in bringing our research team together; we are also grateful for helpful comments from reviewers.

REFERENCES

Abu-Shumays, I. (1966). *Nuclear Science and Engineering*, **26**, 430–431.
Abu-Shumays, I. (1967). *Nuclear Science and Engineering*, **27**, 607–608.
Baker, Jr., G. A. (1975). *Essentials of Padé Approximants*, Academic Press, New York.
Bender, C. and Orszag, S. (1978). *Advanced Mathematical Methods for Scientists and Engineers*, McGraw-Hill, New York.
Chandrasekhar, S. (1960). *Radiative Transfer*, Dover, New York.
Dunn, W. L., Garcia, R. D. M., and Siewert, C. E. (1982). *Astrophysical Journal*, **260**, 849–854.
Ellis, J., Gardi, E., Karliner, M., and Samuel, M. A. (1996). *Physics Letters B*, **366**, 268–275.
Kelley, C. T. (1978). *Journal of Mathematical Physics*, **19**, 500–501.
Kelley, C. T. (1980). *Journal of Mathematical Physics*, **21**, 1625–1628.
Kelley, C. T. (1982). *Journal of Mathematical Physics*, **23**, 2097–2100.
McCormick, N. J. (1979). *Journal of Mathematical Physics*, **20**, 1504–1507.
Samuel, M. A., Ellis, J., and Karliner, M. (1995a). *Physical Review Letters*, **74**, 4380–4383.
Samuel, M. A., Li, G., and Steinfelds, E. (1995b). *Physical Review E*, **51**, 3911–3933.
Sanchez, R., and McCormick, N. J. (1981). *Journal of Mathematical Physics*, **22**, 847–855.

Siewert, C. E. (1978). *Journal of Mathematical Physics,* **19**, 1587–1588.
Siewert, C. E. (1979). *Journal of Quantitative Spectroscopy and Radiative Transfer,* **22**, 441–446.
Stibbs, D. W. N., and Weir, R. E. (1959). *Monthly Notices of the Royal Astronomical Society,* **119**, 512–525.
Vainshtein, A. I., and Zakharov, V. I. (1994). *Physical Review Letters,* **73**, 1207.