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δ-Fit: A fast and accurate treatment of particle scattering phase functions with weighted singular-value decomposition least-squares fitting

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Abstract

With a limited number of polynomial terms (so-called "streams"), there are significant differences between a phase function and its Legendre polynomial expansion at large scattering angles, which are important to satellite observations. This study finds that while it takes hundreds of Legendre polynomial expansion terms to simulate the backscattering portion of cloud phase functions accurately, the backscattered radiance pattern can be accurately estimated with only 30 Legendre polynomial expansion terms by replacing the regular Legendre polynomial expansion coefficients by coefficients obtained by a weighted singular-value decomposition least-squares fitting procedure. Thus the computing time can be significantly reduced. For satellite remote-sensing purposes, the weighted least-squares Legendre polynomial fitting is an optimal estimation of the cloud phase function.

1. Introduction

In current discrete ordinate radiative transfer models [1,2], the scattering phase function of particles is represented by just a few Legendre polynomial expansion terms. The expansion of the phase function in Legendre polynomials has the advantage that in slab geometry the intensity can be represented by a Fourier cosine series, and each expansion coefficient (i.e. intensity component) in the series satisfies an azimuthally independent, integro-differential radiative transfer equation. There is one equation associated with each cosine term, and these equations are uncoupled and mathematically identical. Thus, we can solve each of these equations with the same mathematical

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scheme. In the discrete-ordinate method the number of terms adopted for the expansion of the phase function in Legendre polynomials is usually taken to be the same as the number of angular points used to approximate the integral term in the radiative transfer equation with a quadrature sum (i.e. the number of streams). Since the cpu-time for computing multiply-scattered radiances with the discrete ordinate method is proportional to the third power of the number of streams, accurate radiance computation is difficult to achieve because of the computational burden.

For very small particles (i.e. size parameter much smaller than 1), the scattering phase function can be accurately determined from just a few Legendre polynomial expansion terms. For moderately larger particles, such as cloud droplets, the scattering phase function is strongly forward peaked. The Legendre polynomial series converges very slowly as the number of terms increases because of the δ-function-like forward peak feature.

The Delta-M method [3], which takes advantage of the fact that the higher-order Legendre polynomial expansion terms contribute primarily to the δ-function-like forward peak [4], is a very efficient technique of removing the strong forward-scattering peak and reducing the error resulting from use of a limited number of Legendre polynomial expansion terms (streams). The Delta-M method conserves most moments of a phase function and it provides accurate fluxes for optically thick media. But the Delta-M method can cause problems for radiance computations if there are not enough terms in the expansion. For ice clouds hundreds of Legendre polynomial expansion terms are required to avoid negative phase function values for large scattering angles as well as for angles around 23°. For optically thin media (optical depth less than 1), use of the exact phase function for single and secondary scattering and a few moments of the phase function for multiple scattering calculation gives good accuracy for the radiance fields [5]. However, for optically thicker media, this correction may not be self-consistent.

The biggest differences between a cloud phase function and its representation by a limited number of Legendre polynomial expansion terms occur at large scattering angles, which are important viewing angles for most satellite observations. The Legendre polynomial expansion coefficients are sensitive to phase function changes in the forward-scattering direction because the values of the phase function as well as their derivatives are several orders of magnitude larger than for the backward direction. With a limited number of terms, the Legendre polynomial expansion may not provide the best estimate of a phase function.

In the next section we show that by replacing the usual coefficients in the Legendre polynomial expansions by new coefficients computed from a weighted least-squares fitting procedure, we can reduce the number of streams substantially while improving accuracy as well as computational speed in radiance computations.

2. Improved Legendre polynomial approximation of the phase function: Weighted singular-value decomposition (SVD) least-squares fitting (δ-fit)

2.1. Differences between δ-fit and δ-M

The Legendre polynomial expansion (or approximation) of a phase function is

$$P(\Theta) = \sum_{l=0}^{N} x_l p_l(\cos\Theta), \tag{1}$$

$$x_l = \frac{2}{2l+1}\int_{-1}^{1} p_l(\cos\Theta)P_{\mathrm{ac}}(\Theta)d(\cos\Theta), \tag{2}$$

where x_l is the lth expansion coefficient, p_l is the lth-order Legendre polynomial, $P_{\mathrm{ac}}(\Theta)$ is the actual phase function that we want to approximate as well as possible, and Θ is the scattering angle. A δ-function with an integration value f requires an infinite number of Legendre polynomial expansion terms and all expansion coefficients have the value f. To remove a δ-function-like forward peak, the δ-M method replaces x_l by $(x_l - f)/(1 - f)$,

$$P_{\delta_{\mathrm{M}}}(\Theta) = \sum_{l=0}^{2N-1} \frac{(x_l - f)}{(1-f)} p_l(\cos\Theta), \quad f = x_N. \tag{3}$$

For a limited number of terms N, the phase function computed from Eq. (3) can be very different from the actual phase function. For any given number of terms N, Eq. (3) is not the best Legendre polynomial fitting of the phase function.

The objective of this study is to develop a robust technique which performs a least-squares fitting to generate coefficients c_l of the Legendre polynomial expansion that minimize the relative difference ε between the approximate phase function $P'(\Theta_i)$ and the actual phase function $P_{\mathrm{ac}}(\Theta_i)$:

$$\varepsilon = \sum_i w_i \left(\frac{P'(\Theta_i)}{P_{\mathrm{ac}}(\Theta_i)} - 1 \right)^2, \tag{4}$$

$$P'(\Theta_i) = \sum_{l=0}^{N_{\mathrm{str}}} c_l p_l(\cos\Theta_i), \tag{5}$$

where Θ_i is the scattering angle, w_i is the weight for each scattering angle, $p_l(\cos\Theta_i)$ is the lth-order Legendre polynomial, N_{str} is the number of streams needed in order to achieve a desired accuracy.

Here the expansion coefficients c_l are computed by solving the least-squares fitting problem $\partial\varepsilon/\partial c_k = 0$ $(k = 0, N)$:

$$\sum_{i=0} \frac{p_k(\cos\Theta_i)}{P_{\mathrm{ac}}(\Theta_i)} w_i \left(\sum_{l=0}^{N_{\mathrm{str}}} \frac{c_l p_l(\cos\Theta_i)}{P_{\mathrm{ac}}(\Theta_i)} - 1 \right) = 0. \tag{6}$$

If the weights for the forward-scattering angles (e.g., $\Theta < 3^\circ$) are set to zero, c_0 will not vanish because the forward peak is automatically truncated (δ-function at 0° scattering angle) with truncation factor $f = 1 - c_0$. The normalized phase function $P_{\delta\text{-fit}}(\Theta)$ is

$$P_{\delta\text{-fit}}(\Theta_i) = \frac{1}{1-f} P'(\Theta_i). \tag{7}$$

The advantages of the above method are:

- better estimation of phase function at large scattering angles with small phase function values;
- easy removal of the forward peak by selecting small weights for scattering angles close to zero;
- ability to keep the lowest several moments if needed.

2.2. Fitting the phase function

The procedure adopted to fit the phase function is:

- interpolate the actual phase function $P_{ac}(\Theta)$ to 361 scattering angles Θ_i with half-degree equal intervals;
- select a forward peak removal angle Θ_c. For $\Theta_i < \Theta_c$, $w_i = 0$;
- select an initial number of streams, N_{str}, and compute all required Legendre polynomials $p_l(\cos\Theta_i)$ for $l \leq N_{str}$;
- solve the linear equations $\partial\varepsilon/\partial c_l = 0$ to derive the coefficients c_l with the singular-value decomposition method;
- if ε is larger than expected, increase N_{str} and repeat the above procedures until ε is small enough;
- determine the scaling factor $f = 1 - c_0$ and renormalize the phase function (i.e. divide all c_l by c_0);
- adjust the extinction cross section β and single scattering albedo ω: $\beta' = 1 - \omega f$, $\omega' = (1 - f)\omega(1 - \omega f)^{-1}$ to subtract the removed forward δ-peak [4] from the scattering cross section.

The results can then be compared with the usual Legendre polynomial expansion method as well as the δ-M method:

- Legendre polynomial expansion method: compute all the expansion coefficients x_l from Eq. (2), and normalize the phase function;
- δ-M method: set the scaling factor $f = x_{N_{str}}$, compute δ-M coefficients: $(x_l - x_{N_{str}})/(1 - x_{N_{str}})$ (Eq. (3)), and adjust the extinction cross section and the single scattering albedo as indicated above.

Since the scattering phase function changes from 0.001 to ∞, it is crucial to treat the interpolation and integration properly. The 180° scattering angles are divided into 18 angular intervals and for each interval we use 20 Lobatto quadrature points and weights for the integration. A four-point Lagrange interpolation scheme is adopted to take the curvature into account.

Since elements of the matrix to be inverted for the least-squares fitting can differ by several orders of magnitude, the singular-value decomposition method is applied for the matrix inversion to overcome possible computer accuracy problems. Eigenvalues which are 10^{-6} times smaller than the largest eigenvalue are considered to be zero.

3. Comparisons of phase functions and reflected radiance fields

3.1. Radiative transfer calculations

The radiances for the full phase functions are computed from Monte-Carlo simulations. The radiances for the scaled phase functions are computed from a discrete ordinate method [2]. The incident flux is π. Optical depth, τ, is 3 and single scatter albedo, ω, is 1 for the comparisons. The solar zenith angle is 0°. Similar studies are also performed for other values of τ, ω and sun angle.

3.2. Henyey–Greenstein phase function

The Legendre polynomial expansion of the Henyey–Greenstein (H–G) phase function is

$$P_{\mathrm{HG}}(\Theta) = \sum_{l=0}^{N} g^l p_l(\cos\Theta), \tag{8}$$

where g is the asymmetry factor and g^l is the lth expansion coefficent as defined by Eq. (3). There are three H–G phase functions with $g = 0.85$ in the top panel of Fig. 1:

- the actual (or true) H–G phase function ($N = \infty$) (solid line);
- the δ-fit to the H–G phase function (obtained by using $N_{\mathrm{str}} = 16$ and by replacing the ususal Legendre polynomial coefficients g^l by the coefficients derived from the least-squares fits) (dashed line); and
- the Delta-M approximation to the H–G phase function ($N = 16$ with δ-M) (dotted line).

The middle panel shows the relative errors of the δ-fit and the δ-M phase functions. The corresponding radiance fields are provided in the lower panel.

At backscatter angles the values of the δ-fit phase function are essentially the same as for the actual (true) phase function. The δ-M phase function fluctuates around the true phase function. The relative error increases with the scattering angle (middle panel of Fig. 1).

The reflected radiances resulting from use of the δ-fit phase function are the same as the true values resulting from use of the true phase function, while the radiances resulting from use of the δ-M phase function are slightly different from the true radiances.

3.3. Double H–G phase function

Most particle scattering phase functions have both forward and backward peaks, which can be simulated as a double H–G phase function:

$$P_{\mathrm{dHG}}(\Theta) = \sum_{l=0}^{N} (F g_1^l + (1 - F) g_2^l) p_l(\cos\Theta), \tag{9}$$

where g_1 and g_2 represent forward and backward peaks, respectively ($g_1 > 0$, $g_2 < 0$). Here $g_1 = 0.92$, $g_2 = -0.7$, $F = 0.98$.

The reflected radiance errors for the δ-fit method are almost zero (Fig. 2). The reflected radiance errors for δ-M method can be as large as 20%.

3.4. Water cloud (Mie scattering) phase function

Fig. 3 is a typical water cloud phase function at near-infrared region with effective droplet size 10 μm. The side scattering area of the phase function was not properly represented with the δ-M method (28 terms of Legendre polynomial expansion). It also does not generate a backscattering peak at the scattering angle of 180°. Replacing the Legendre usual expansion coefficients by the coefficients obtained from use of the least-squares δ-fit, the phase functions and radiances in the backscatter directions are the same as the exact values.

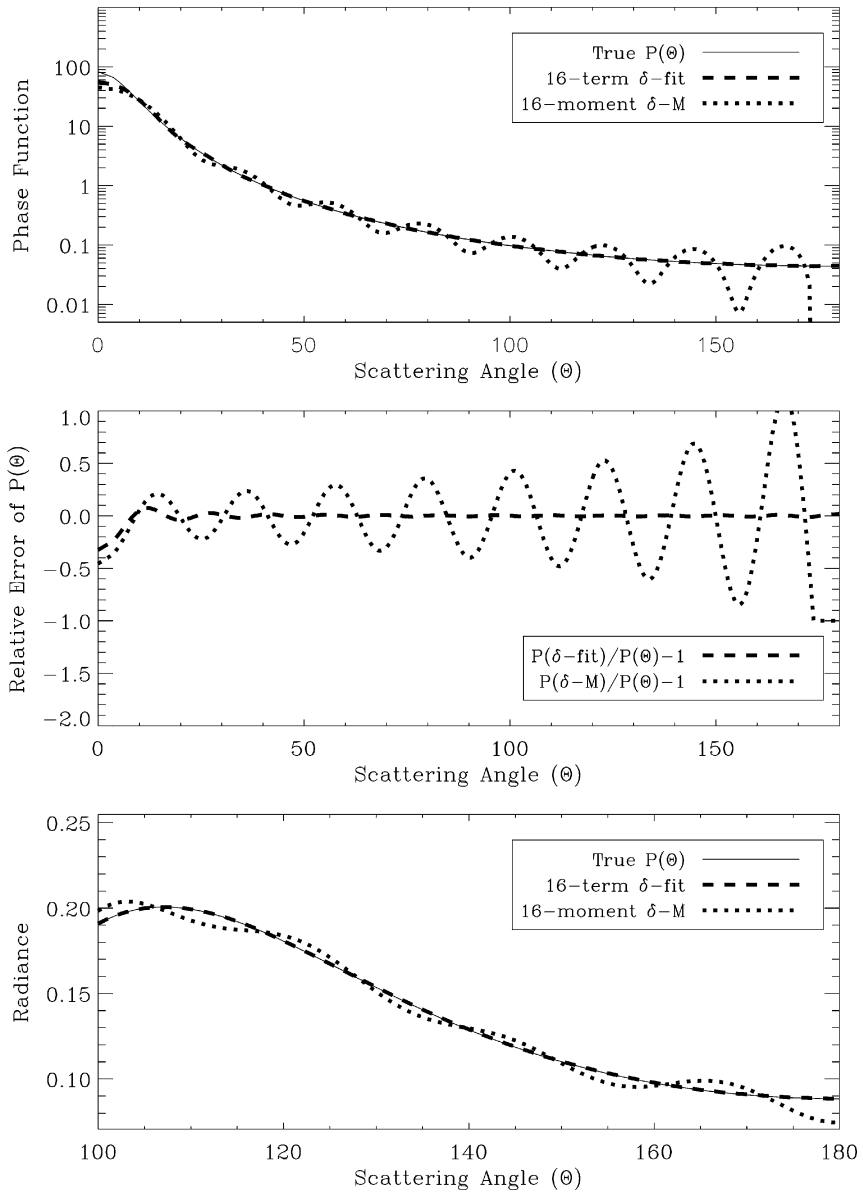

Fig. 1. H–G phase functions ($g = 0.85$) (top panel), differences among them (middle panel) and radiances (bottom panel): original phase function (solid), δ-fit: 16 term Legendre polynomial fits (dash), δ-M: 16 moments of Legendre polynomial expansion (dot).

3.5. *Ice cloud scattering phase function*

The ice cloud phase function [6] has a sharp forward peak, a 23° halo and a 180° backscattering peak (Fig. 4). Using the δ-fit method, the phase function as well as the reflected radiances are the same as for the true phase function. Again, the δ-M method failed to generate a good backward peak.

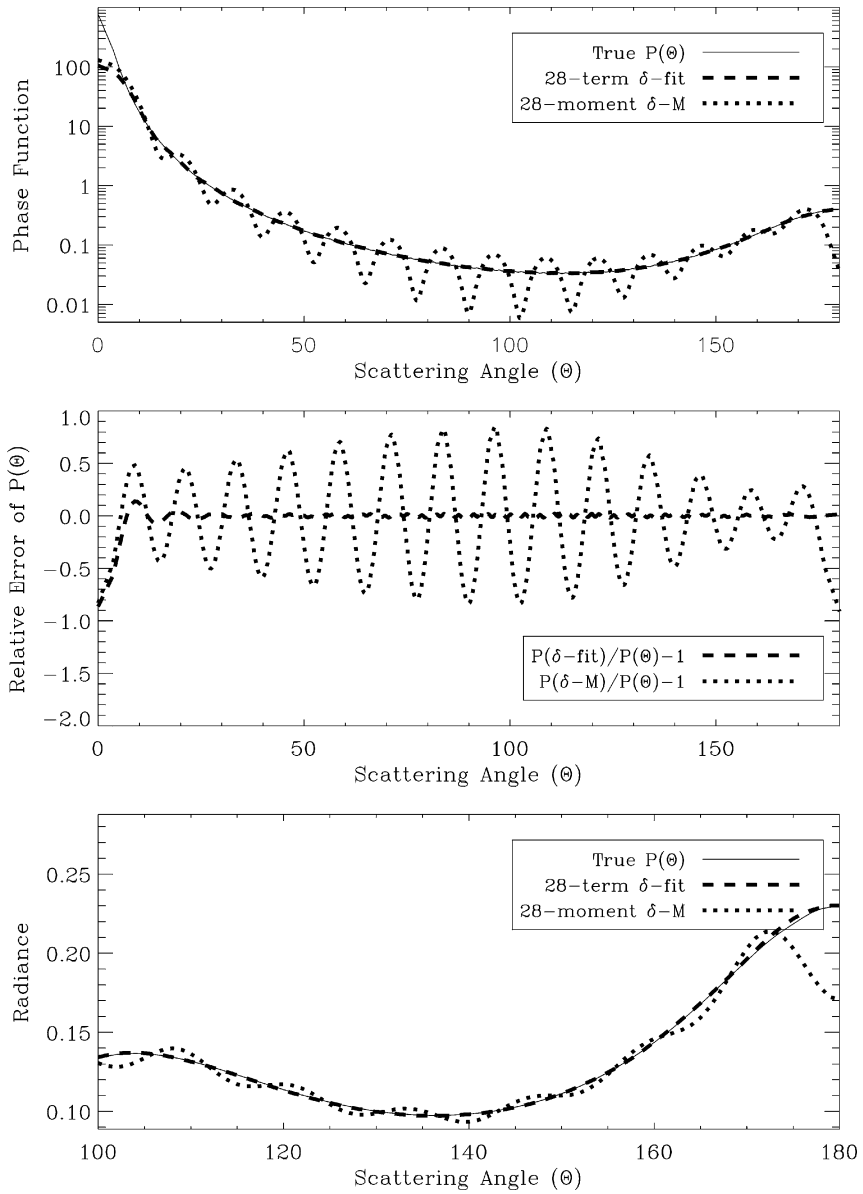

Fig. 2. Double H–G phase functions ($F = 0.98$, $g_1 = 0.92$, $g_2 = -0.7$) (top panel) differences among them (middle panel) and radiances (bottom panel): original phase function (solid), δ-fit: 28 term Legendre polynomial fits (dash), δ-M: 28 moments of Legendre polynomial expansion (dot).

4. Summary and discussions

A δ-fit method is developed for fast and accurate computation of reflected radiances. In contrast to the δ-M method, which conserves most of the Legendre moments of a phase function, the δ-fit

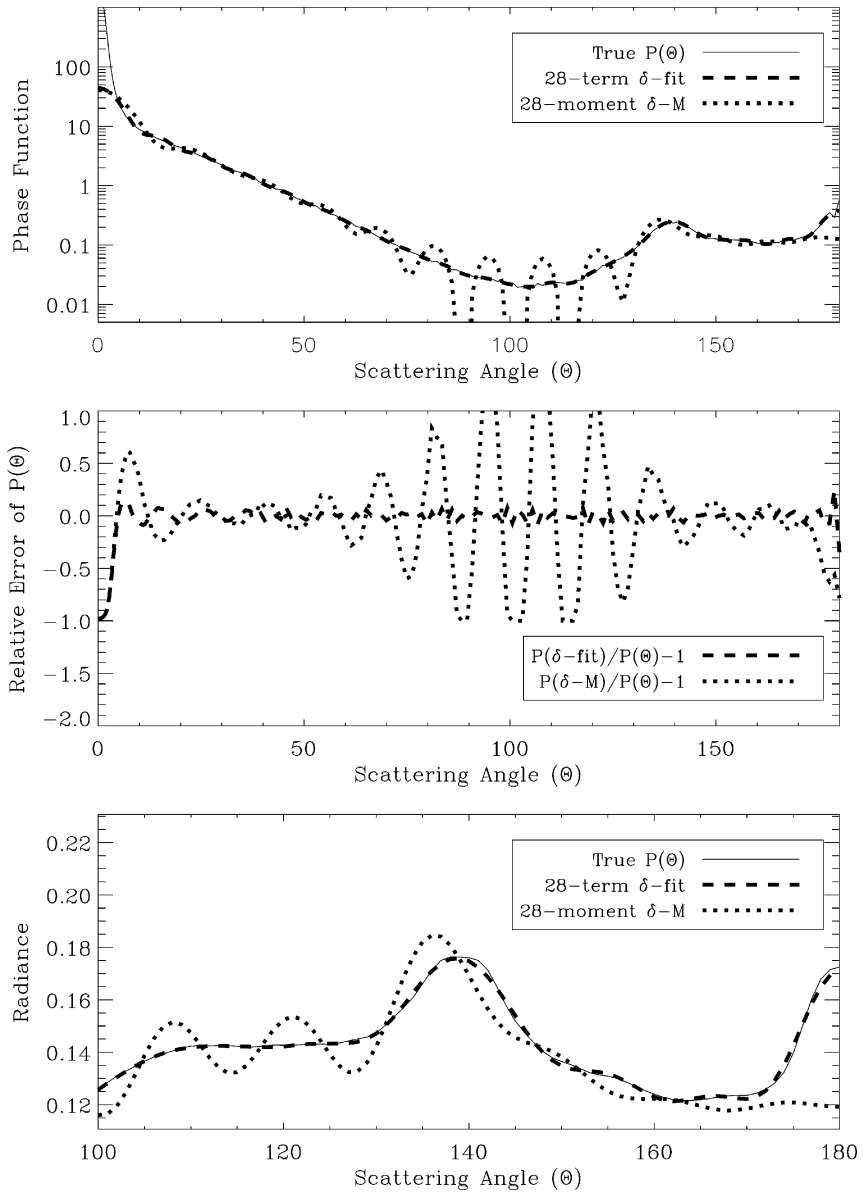

Fig. 3. Water cloud phase functions (for $\lambda = 1.6$ μm, $R_e = 10$ μm) (top panel) differences among them (middle panel) and radiances (bottom panel): original phase function (solid), δ-fit: 28 term Legendre polynomial fits (dash), δ-M: 28 moments of Legendre polynomial expansion (dot).

method conserves only the lowest several moments and derives the rest of Legendre polynomial coefficients through a least-squares fitting procedure. The least-squares method is weighted by the relative error for each scattering angle and thus has a good representation of the backscattering angles.

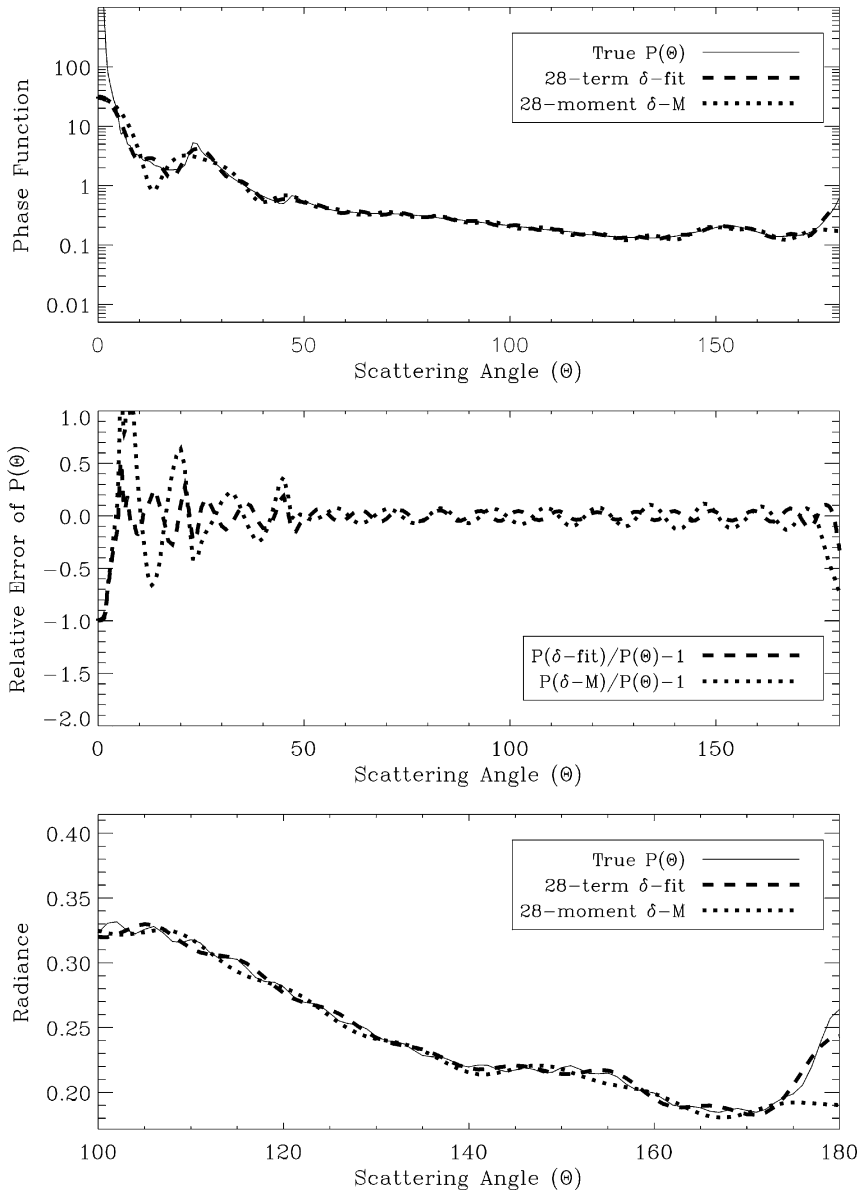

Fig. 4. Ice cloud phase functions (for $\lambda = 0.55$ μm, $D_e = 20$ μm) (top panel) differences among them (middle panel) and radiances (bottom panel): original phase function (solid), δ-fit: 28 term Legendre polynomial fits (dash), δ-M: 28 moments of Legendre polynomial expansion (dot).

Using the new method, we can accurately compute the reflected radiances with less than 30 streams for both water and ice clouds. This method is suitable for all optical depths.

A computer code which generates the least-squares fits as well as all moments of Legendre polynomial expansion for any given phase function is available to the community through our web site at http://adm.larc.nasa.gov/yhu/phasefit.

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