A Polarized Delta-Four-Stream Approximation for Infrared and Microwave Radiative Transfer: Part I

K. N. LIOU, S. C. OU, AND Y. TAKANO

Department of Atmospheric and Oceanic Sciences, University of California, Los Angeles, Los Angeles, California

Q. LIU

Joint Center for Satellite Data Assimilation, NOAA, Camp Springs, Maryland

(Manuscript received 23 July 2004, in final form 29 November 2004)

ABSTRACT

The delta-four-stream polarized (vector) thermal radiative transfer has been formulated and numerically tested specifically for application to satellite data assimilation in cloudy atmospheres. It is shown that for thermal emission in the earth’s atmosphere, the \([I, Q]\) component of the Stokes vector can be decoupled from the \([U, V]\) component and that the solution of the vector equation set involving the four-stream approximation can be expressed in an analytic form similar to the scalar case. Thus, the computer time requirement can be optimized for the simulation of forward radiances and their derivatives. Computations have been carried out to illustrate the accuracy and efficiency of this method by comparing radiance and polarization results to those computed from the exact doubling method for radiative transfer for a number of thermal infrared and microwave frequencies. Excellent agreement within 1% is shown for the radiance results for all satellite viewing angles and cloud optical depths. For polarization, differences between the two are less than 5% if brightness temperature is used in the analysis. On balance of the computational speed and accuracy, the four-stream approximation for radiative transfer appears to be an attractive means for the simulation of cloudy radiances and polarization for research and data assimilation purposes.

1. Introduction

Satellite data assimilation requires an efficient and accurate radiative transfer model for the computation of radiances and the associated derivatives. The thermal radiative transfer model that has been used for data assimilation in numerical weather prediction models was primarily developed for clear conditions, that is, for pure absorbing atmospheres, such that the atmospheric transmittance and the gradient of radiance relative to a state variable are parameterized or derived analytically. However, more than 50% of the satellite data are contaminated by clouds, thus making the incorporation of scattering effects in transmittance calculations an important but challenging issue. In the microwave region, polarization is a significant factor affecting the transfer of radiation in the surface–atmosphere system (Liu and Weng 2002; Weng and Liu 2003). In view of the fact that many advanced infrared and microwave sensors have been and will be built and deployed in space, it is essential to develop an accurate radiative transfer model that can be effectively applied to cloudy atmospheres for satellite data assimilation and to test its impact in terms of the improvement of forecast models (Matricardi et al. 2004; Chevallier et al. 2004).

In our previous work, we presented a systematic development of the delta-four-stream (D4S) approximations for radiative transfer, specifically designed for application to cloudy and aerosol atmospheres (Liou et al. 1988; Liou 2002). We demonstrated that an analytic solution for this approximation can be derived explicitly for homogeneous layers with a minimal computational effort for flux calculations. Fu and Liou (1993) have shown that D4S can achieve an excellent accuracy in spectral radiative flux calculations for a wide range of cloud optical depth, single-scattering albedo, and the phase-function expansion terms. However, our D4S method has been derived for the intensity (or radiance) component without accounting for polarization. The transfer of thermal infrared radiation in the earth’s atmosphere generates little polarization, except in high-
level clouds that contain horizontally oriented ice crystals (Takano and Liou 1993). But the transfer of microwave radiation is highly polarized, particularly over the ocean surfaces.

In this paper, we first formulate the basic equations governing the transfer of the Stokes vector in a plane-parallel atmosphere for thermal emission. We show that, for thermal emission in the earth’s atmosphere, it suffices to use the $I$ and $Q$ components of the Stokes vector in polarization analysis, as presented in section 2. In section 3, we formulate the four-stream approximation for polarized thermal radiative transfer in which the elements in the scattering phase matrix are expanded into four terms in line with the four radiative streams. The solution of a set of differential equations is expressed in terms of a homogeneous plus a particular solution. Eigenvalues associated with the solution, critical in the four-stream analysis, are determined by an efficient numerical scheme. Section 4 contains some computational results for illustration of the accuracy and speed of the D4S method in comparison to exact calculations based on the doubling method, discussed in this section. Summary is given in section 5.

2. Formulation of polarized thermal radiative transfer and the phase matrix

The basic equation governing the transfer of the Stokes vector, \( \mathbf{I} = [I, Q, U, V] \), in a plane-parallel atmosphere for thermal emission can be expressed in the form (see, e.g., Takano and Liou 1993)

\[
\mu \frac{d\mathbf{I}(\tau, \mu, \phi)}{d\tau} = \mathbf{I}(\tau, \mu, \phi) - \mathbf{J}(\tau, \mu, \phi),
\]

where \( \mu = \cos \theta \), \( \theta \) is the zenith angle, \( \phi \) is the azimuthal angle, \( \tau \) is the optical depth, and the source function is given by

\[
\mathbf{J}(\tau, \mu, \phi) = \frac{\sigma}{4\pi} \int_{-1}^{1} \mathbf{Z}(\mu, \mu', \phi') \mathbf{I}(\tau, \mu', \phi') d\mu' + (1 - \sigma) \mathbf{B},
\]

(1a)

where \( \sigma \) is the single-scattering albedo, \( \mathbf{B} \) is the Planck function vector \( [B_\nu(T), 0, 0, 0] \), \( T \) is temperature, \( \nu \) is wavenumber, and the phase matrix with respect to the local meridian plane is defined in the form

\[
\mathbf{Z}(\mu, \mu', \phi') = \mathbf{L}(\pi - i_2) \mathbf{P}(\theta) \mathbf{L}(-i_1),
\]

(2)

with \( \mathbf{L}(\pi - i_2) \) and \( \mathbf{L}(-i_1) \) the linear transform matrices, which are required to rotate the meridian plane containing the incident and outgoing vectors to the scattering plane (Hovenier 1969). In general, the scattering phase matrix, \( \mathbf{P} \), contains 16 nonzero elements.

For a plane-parallel atmosphere, the emitted thermal radiation from the surface and the atmosphere is symmetrical with respect to the azimuthal angle. Thus, we can perform azimuthal average over \( \phi \) to obtain

\[
\mu \frac{d\mathbf{I}(\tau, \mu)}{d\tau} = \mathbf{I}(\tau, \mu) - \mathbf{J}(\tau, \mu),
\]

(3)

where the azimuthally averaged source function can be written in the form

\[
\mathbf{J}(\tau, \mu) = \frac{\sigma}{\pi} \int_{-1}^{1} \mathbf{Z}(\mu, \mu') \mathbf{I}(\tau, \mu') d\mu' + (1 - \sigma) \mathbf{B}.
\]

(3a)

The azimuthally averaged phase matrix \( \mathbf{Z}(\mu, \mu') \) is given by

\[
\mathbf{Z}(\mu, \mu') = \frac{1}{2\pi} \int_{0}^{2\pi} \mathbf{Z}(\mu, \phi, \mu', \phi') d(\phi - \phi').
\]

(4)

The phase matrix inside the integral is the product of three terms denoted in Eq. (2). Each term can be expanded in terms of the Fourier series. Because of the orthogonal properties of sine and cosine functions in the expansion, we can prove that \( Z_{ij} = 0 \) for \( i, j = 13, 14, 23, 24, 31, 32, 41, \) and \( 42 \). In this manner, the Stokes vector, \( [I, Q, U, V] \), can be decomposed into \( [I, Q] \) and \( [U, V] \) independently. Van de Hulst (1980, chapter 15) also discussed the expansion of the phase matrix elements using the Fourier series and presented equations for them in terms of sine and cosine. The emitted Stokes vector from clouds and the surface generally contains only the \( [I, Q] \) component and thus we can safely neglect the \( [U, V] \) component for analysis of the polarized thermal radiative transfer. We can then use \( [I, Q] \) in the analysis of the transfer of polarized radiation, as described in Takano and Liou (1993). Thus, the 2 by 2 phase matrix elements can now be expressed as follows:

\[
\mathbf{Z} = [Z_{ij}(\mu, \mu')]_{2 \times 2} = \left[ \begin{array}{cc} P_{11}^{ij} & P_{12}^{ij} \cos 2i_1 \\ P_{21} \cos 2i_2 & P_{22} \cos 2i_1 \cos 2i_2 - P_{33} \sin 2i_1 \sin 2i_2 \end{array} \right],
\]

(5)

where the bars represent the azimuthally averaged value. We can further expand this matrix \( \mathbf{Z} \) in terms of the associated Legendre polynomial \( P_n^m(\mu) \) in the form

\[
Z_{ij}(\mu, \mu') = \sum_{m=0}^{N} \sum_{l=m}^{N} (\overline{\sigma}_{ij})_m^n P_n^m(\mu) P_n^m(\mu'),
\]

(6)

where \( (\overline{\sigma}_{ij})_m^n \) are the expansion coefficients averaged over the relative azimuthal angle \( \phi - \phi' \). Details on the derivation of Eq. (6) along with the expressions for \( (\overline{\sigma}_{ij})_m^n \) are given in appendix A. The \( Z_{ij}(\mu, \mu') \) values calculated from Eq. (6) are identical to those determined on the basis of a direct azimuthal averaging according to Eq. (5). Note that we require these coefficients to develop the four-stream approximation.
To simplify the radiative transfer equation, we define
\[
\mathbf{b}_{ij} = \begin{cases} 
\mathbf{c}_i/\mu_j, & i \neq j \\
(\mathbf{c}_i - \mathbf{E})/\mu_j, & i = j 
\end{cases} 
\]  
(7)
\[
\mathbf{c}_{ij} = \frac{\mathbf{e}}{2} a_i \sum_{m=0}^{N} \sum_{l=-m}^{N} \left[ \begin{array}{c}
(\mathbf{w}_{11}^m) I_l^m \\
(\mathbf{w}_{21}^m) I_l^m
\end{array} \right] P_i^m(\mu_l) P_j^m(\mu_l),
\]  
(8)
where \( \mathbf{E} \) is the \( 2 \times 2 \) identity matrix and \( a_i \) are the Gaussian quadrature weights. Based on the property of Legendre polynomials, we find the following symmetric relationships:
\[
\mathbf{b}_{i-j} = -\mathbf{b}_{i+j}, \quad \mathbf{b}_{i-j} = -\mathbf{b}_{i-j}.
\]  
(9)
These symmetry relationships have also been discussed by de Haan et al. (1987) and Hovenier and van der Mee (1983). By replacing the integral by summation according to the Gaussian quadrature and using the phase matrix expansion expressed in Eq. (6), we can decompose Eq. (1) into \( 4 \times n \) linear first-order differential equations in the form
\[
\begin{bmatrix}
I_{-2} \\
Q_{-2}
\end{bmatrix}
\begin{bmatrix}
\mathbf{I} \\
\mathbf{Q}
\end{bmatrix}
+ \begin{bmatrix}
I_{-1} \\
Q_{-1}
\end{bmatrix}
\begin{bmatrix}
I_1 \\
Q_1
\end{bmatrix}
+ \begin{bmatrix}
I_2 \\
Q_2
\end{bmatrix}
\begin{bmatrix}
S_{-21} \\
S_{-22}
\end{bmatrix}
= \begin{bmatrix}
(\mathbf{b}_{2,2})_{11} \\
(\mathbf{b}_{2,2})_{12} \\
(\mathbf{b}_{2,2})_{21} \\
(\mathbf{b}_{2,2})_{22}
\end{bmatrix}
\begin{bmatrix}
(\mathbf{S}_{11})_{11} \\
(\mathbf{S}_{11})_{12} \\
(\mathbf{S}_{12})_{11} \\
(\mathbf{S}_{12})_{12}
\end{bmatrix}
\]  
(10)
where \( n \) is the number of upward and downward streams and the source term is given by
\[
\begin{bmatrix}
(\mathbf{S}_{11}) \\
(\mathbf{S}_{12})
\end{bmatrix}
= \begin{bmatrix}
1 - \mathbf{e} \\
0
\end{bmatrix}
\begin{bmatrix}
B_s(T)/\mu_i \\
0
\end{bmatrix},
\]  
(11)

3. Four-stream approximation for polarized thermal radiative transfer

We consider two radiative streams in the upper and lower hemisphere (i.e., \( n = 2 \)). At the same time, we expand the scattering phase matrix in four terms (\( N = 3 \)) so that the total number of streams is equal to the total number of phase matrix expansion terms, a mathematical requirement in the discrete-ordinates method for radiative transfer (Chandrasekhar 1950). Using the relation denoted in Eq. (9), eight first-order differential equations can then be written in matrix form as follows:

\[
\begin{bmatrix}
I_{-2} \\
Q_{-2} \\
I_{-1} \\
Q_{-1} \\
I_1 \\
Q_1 \\
I_2 \\
Q_2
\end{bmatrix}
\begin{bmatrix}
S_{-21} \\
S_{-22} \\
S_{-11} \\
S_{-12} \\
S_{11} \\
S_{12} \\
S_{21} \\
S_{22}
\end{bmatrix}
= \begin{bmatrix}
(\mathbf{b}_{2,2})_{11} \\
(\mathbf{b}_{2,2})_{12} \\
(\mathbf{b}_{2,2})_{21} \\
(\mathbf{b}_{2,2})_{22}
\end{bmatrix}
\begin{bmatrix}
(\mathbf{S}_{11})_{11} \\
(\mathbf{S}_{11})_{12} \\
(\mathbf{S}_{12})_{11} \\
(\mathbf{S}_{12})_{12}
\end{bmatrix}
\]  
(12)
The conventional Gauss quadratures and weights in the four-stream approximation are \( \mu_1 = 0.339 \, 981 \) and \( \mu_2 = 0.861 \, 136 \), and \( a_1 = 0.652 \, 145 \) and \( a_2 = 0.347 \, 854 \). However, because of the isotropic emission source in the thermal IR and microwave radiative transfer, the double Gauss quadratures and weights \( (\mu_1 = 0.211 \, 324 \, 8 \) and \( \mu_2 = 0.788 \, 675 \, 2 \), and \( a_1 = a_2 = 0.5 \)) have the advantage of producing higher accuracy in intensity calculations. The \( 8 \times 8 \) matrix in Eq. (12) represents the coupled multiple-scattering contribution to the \( I \) and \( Q \) components.

To find eigenvalue and eigenvector matrices for Eq. (12), we define the sum and difference for the upward and downward intensity vectors in the form

\[
M_{1,2}^\pm = \begin{pmatrix} I_{1,2}^\pm \\ Q_{1,2}^\pm \end{pmatrix} = \begin{pmatrix} I_{1,2} \mp Q_{1,2} \\ Q_{1,2} \mp Q_{1,2} \end{pmatrix}.
\]

Following some algebraic manipulation, Eq. (12) can be converted into the following four matrix equations:

\[\frac{dM_{1,2}^\pm}{d\tau} = b_{1,2}^\pm M_{1,2}^\pm - S_{1,2}^\pm,\]

(14)

\[\frac{dM_{1,2}^\pm}{d\tau} = b_{1,2}^\pm M_{1,2}^\pm - S_{1,2}^\pm,\]

(15)

where the coefficient matrices are defined by

\[
b_{1,2}^\pm = \begin{pmatrix} (b_{1,2}^\pm)_{11} & (b_{1,2}^\pm)_{12} \\ (b_{1,2}^\pm)_{21} & (b_{1,2}^\pm)_{22} \end{pmatrix},
\]

(16)

and the modified source term is given by

\[
S_{1,2}^\pm = \begin{pmatrix} S_{1,2}^\pm \\ S_{1,2}^\pm \end{pmatrix} = \begin{pmatrix} S_{1,2}^\pm \\ S_{1,2}^\pm \end{pmatrix}.
\]

(17)

Differentiating both sides of Eqs. (14) and (15) yields the following second-order differential equation set:

\[\frac{d^2}{d\tau^2} \begin{pmatrix} M_{1,2}^\pm \\ M_{1,2}^\pm \end{pmatrix} = \begin{pmatrix} a_{22} & a_{21} \\ a_{12} & a_{11} \end{pmatrix} \begin{pmatrix} M_{1,2}^\pm \\ M_{1,2}^\pm \end{pmatrix} + \begin{pmatrix} d_2 \\ d_1 \end{pmatrix},\]

(18a)

where

\[
a_{22} = b_{22}b_{12}^+ + b_{21}b_{12}^+, \quad a_{21} = b_{22}b_{21}^+ + b_{21}b_{11}^+, \quad a_{12} = b_{12}b_{22}^+ + b_{12}b_{12}^+, \quad a_{11} = b_{12}b_{21}^+ + b_{12}b_{11}^+ \]

(18b)

\[
d_1 = S_{2,1} + S_{1,1}, \quad d_2 = S_{2,2} + S_{1,1}.
\]

(18c)

Further differentiation of Eq. (18a) leads to two fourth-order vector differential equations in terms of \( M_{1,2}^\pm \) and \( M_{1,2}^\pm \) separately as follows:

\[\frac{d^4}{d\tau^4} M_{1,2}^\pm = a_{i,2} \frac{d^2}{d\tau^2} M_{1,2}^\pm + b_i M_{1,2}^\pm + c_i, \quad i = 1, 2,\]

(19a)

where

\[
a_1 = a_{11} + a_{12}a_{22}a_{12}^{-1}, \quad a_2 = a_{22} + a_{21}a_{11}a_{21}^{-1},
\]

(19b)

\[
b_1 = a_{12}a_{21} - a_{12}a_{22}a_{12}^{-1}a_{11},
\]

(19c)

\[
b_2 = a_{22}a_{12} - a_{21}a_{11}a_{21}^{-1}a_{22},
\]

(19d)

The complete solution for \( M_{1,2}^\pm \) is composed of a homogeneous and a particular solution. Thus,

\[\begin{pmatrix} M_{1,2}^\pm \\ M_{1,2}^\pm \end{pmatrix} = \sum_{j=-2}^{2} \begin{pmatrix} \exp(-k_j\tau) & 0 \\ 0 & \exp(-k_j\tau) \end{pmatrix} \begin{pmatrix} G_{1j} \\ G_{1j} \end{pmatrix} + \begin{pmatrix} \eta_2 \\ \eta_1 \end{pmatrix},\]

(20a)

where \( G_{1j} \) is a vector associated with the \( j \)th quadrature angle and the \( j \)th eigenvalue, \( \eta \) is the particular solution vector for \( M_{1,2}^\pm \), and the term

\[\exp(-k_j\tau) = R \begin{pmatrix} \exp(-(k_j)_{1,2}\tau) & 0 \\ 0 & \exp(-(k_j)_{2,1}\tau) \end{pmatrix} R^{-1},\]

(20b)

where \( R \) and \( R^{-1} \) are the eigenvector matrix and its inverse, respectively, and \( (k_j)_{1,2} \) and \( (k_j)_{2,1} \) are the \( j \)th set of eigenvalues. On substituting Eq. (20a) into Eq. (19a), we obtain a set of characteristic matrix equations for the solution of eigenvalues and a set of relationships for determining the particular solutions. The particular solutions are

\[
\eta_2 = -c_2^{-1}(a_2, d_1 - a_{2,1}a_{1,2}^+d_2),
\]

(21a)

\[
\eta_1 = -c_1^{-1}(a_1d_2 - a_{1,2}a_{1,2}^+d_1).
\]

(21b)

The characteristic equation is given by

\[\sum_{j=-2}^{2} (k_j^4 - a_i k_j^2 - b_i) \exp(-k_j\tau) G_{1j} = 0, \quad i = 1, 2,\]

(22)

To have nontrivial solutions for \( G_{1j} \), we must have

\[f(k) = k^4 - a_i k^2 - b_i = 0, \quad i = 1, 2,\]

(23)

By setting each element of \( f(k) \) to 0 leads to four algebraic equations. Although Eq. (22) appears to be quadratic, it cannot be solved using the quadratic formula,
as having been done in the scalar delta-four-stream method (Liou 2002). For this reason, we have developed a Newton–Raphson numerical iteration method for the solution of eigenvalues \( \mathbf{k}^2 \), which is given in appendix B.

Since \( \mathbf{G}_{ij} \) and \( \mathbf{G}_{2j} \) in Eq. (20) are defined from high-order differentiations, they are mutually dependent. We can determine their relationship from the homogeneous part of Eq. (18a). A straightforward substitution yields

\[
\exp(-k_{11} \tau)\mathbf{G}_{11} + \exp(k_{11} \tau)\mathbf{G}_{1,-1} = \mathbf{A}_i \exp(-k_{21} \tau)\mathbf{G}_{21} + \exp(k_{21} \tau)\mathbf{G}_{2,-1},
\]

\[
\exp(-k_{22} \tau)\mathbf{G}_{12} + \exp(k_{22} \tau)\mathbf{G}_{1,-2} = \mathbf{A}_i \exp(-k_{22} \tau)\mathbf{G}_{22} + \exp(k_{22} \tau)\mathbf{G}_{2,-2},
\]

where \( \mathbf{A}_i = \left(a_{ij} \mathbf{k}_{ij}^2 - \mathbf{a}_{ij}\right), i = 1, 2, \) and \( \mathbf{k}_{ij} \) are the eigenvalue solutions of Eq. (23). Following the same procedure as in the case of Eq. (19a), we can obtain the fourth-order differential equations for \( \mathbf{M}_{ij} \) in the form

\[
\frac{d^4 \mathbf{M}_{ij}}{d \tau^4} = \mathbf{a}_i \frac{d^4 \mathbf{M}_{ij}}{d \tau^4} + \mathbf{b}_i \mathbf{M}_{ij}, \quad i, j = 1, 2.
\]

where the expressions for the coefficients \( \mathbf{a}_i \) and \( \mathbf{b}_j \) are the same as those of \( \mathbf{a}_i \) and \( \mathbf{b}_j \) given in Eqs. (19a)–(19d), except that the superscripts + and − in Eqs. (18a)–(18d) are replaced by − and +, respectively. It is noted that there are no particular solutions for \( \mathbf{M}_{1,2} \), because the source terms are eliminated during the differentiating process. Substituting Eq. (20) into Eqs. (14) and (15), and assuming that the homogeneous solutions for \( \mathbf{M}_{1,2} \), are similar to the homogeneous part of Eq. (20a), we obtain

\[
\mathbf{M}_{j}^{(0)} = (\mathbf{a}^{-})^{-1} \sum_{j=1}^{2} [(\mathbf{b}_{j1})^{-1} \mathbf{A}_i - (\mathbf{b}_{j2})^{-1} \mathbf{k}_{ij}],
\]

\[
\mathbf{M}_{j}^{(0)} = (\mathbf{a}^{-})^{-1} \sum_{j=1}^{2} [(\mathbf{b}_{j2})^{-1} - (\mathbf{b}_{j1})^{-1} \mathbf{A}_i] \mathbf{k}_{ij},
\]

where \( \mathbf{a}^{-} = (\mathbf{b}_{j1})^{-1} \mathbf{b}_{j2} - (\mathbf{b}_{j2})^{-1} \mathbf{b}_{j1} \) and \( \mathbf{a}^{+} = (\mathbf{b}_{j1})^{-1} \mathbf{b}_{j1} - (\mathbf{b}_{j2})^{-1} \mathbf{b}_{j2} \).

Finally, by combining Eqs. (20a), (24), (25), (27), and (28), the complete solutions for \( \mathbf{I}_i = [I_i, Q_i] \) \((i = -2, -1, 1, 2)\) are given by

\[
\begin{bmatrix}
I_1 \\
I_{1-1} \\
I_2 \\
I_{2-1}
\end{bmatrix} =
\begin{bmatrix}
\Phi_{j1}^{+} \exp(-k_{21}\tau) & \Phi_{j1}^{-} \exp(k_{21}\tau) & \Phi_{j2}^{+} \exp(-k_{22}\tau) & \Phi_{j2}^{-} \exp(k_{22}\tau)
\end{bmatrix}
\begin{bmatrix}
\mathbf{G}_{2,1} \\
\mathbf{G}_{2,-1} \\
\mathbf{G}_{2,2} \\
\mathbf{G}_{2,-2}
\end{bmatrix}
\begin{bmatrix}
\eta_1 \\
\frac{1}{2} \eta_1 \\
\eta_2 \\
\frac{1}{2} \eta_2
\end{bmatrix},
\]

Equation (29) then contains four sets of integration constants \( \mathbf{G}_{2,1}, \mathbf{G}_{2,-1}, \mathbf{G}_{2,2}, \mathbf{G}_{2,-2} \). These integration constants are to be determined from boundary conditions. Consider a homogeneous layer having an optical depth \( \tau_1 \). We may assume that there is no diffuse radiation from either the top or the bottom of this layer so that the boundary conditions are

\[
\begin{aligned}
I_{1,-2}(\tau = 0) &= \mathbf{0} \\
I_{1,2}(\tau = \tau_1) &= \mathbf{0}.
\end{aligned}
\]

Substituting Eq. (33) into Eq. (29), we obtain the following equation for the solution of the four integration constants:

\[
\begin{bmatrix}
I_{1,-2} \\
I_{1,2}
\end{bmatrix}
\]

\[
\begin{bmatrix}
\mathbf{G}_{2,1} \\
\mathbf{G}_{2,-1} \\
\mathbf{G}_{2,2} \\
\mathbf{G}_{2,-2}
\end{bmatrix}
\begin{bmatrix}
\eta_1 \\
\frac{1}{2} \eta_1 \\
\eta_2 \\
\frac{1}{2} \eta_2
\end{bmatrix},
\]

where the eigenvector matrices are

\[
\phi_{j1}^{(+)} = \frac{1}{2} \left[ \mathbf{E} \pm (\mathbf{a}^{-})^{-1}[(\mathbf{b}_{j1})^{-1} - (\mathbf{b}_{j2})^{-1} \mathbf{A}_j] \mathbf{k}_{ij} \right],
\]

\[
\phi_{j2}^{(+)} = \frac{1}{2} \left[ \mathbf{A}_j \pm (\mathbf{a}^{-})^{-1}[(\mathbf{b}_{j2})^{-1} - (\mathbf{b}_{j1})^{-1} \mathbf{A}_j] \mathbf{k}_{ij} \right].
\]

To circumvent computational overflow problems, we remove the positive exponential terms in Eq. (29) and define new coefficient vectors \( \mathbf{G}_{2,-1}^{'} \) and \( \mathbf{G}_{2,-2}^{'} \) in the forms

\[
\mathbf{G}_{2,-1}^{'} = \exp(k_{21}\tau)\mathbf{G}_{2,-1}, \quad \mathbf{G}_{2,-2}^{'} = \exp(k_{22}\tau)\mathbf{G}_{2,-2}.
\]
\[
\begin{bmatrix}
0 \\
0 \\
0 \\
0 \\
\end{bmatrix} = \begin{bmatrix}
\Phi_1^+ \exp(-k_{21} \tau) & \Phi_1^- & \Phi_2^+ \exp(-k_{22} \tau) & \Phi_2^- \\
\Phi_1^- & \Phi_1^+ \exp(-k_{21} \tau) & \Phi_2^- & \Phi_2^+ \exp(-k_{22} \tau) \\
\phi_1^+ \exp(-k_{21} \tau) & \phi_1^- & \phi_2^+ \exp(-k_{22} \tau) & \phi_2^- \\
\phi_1^- & \phi_1^+ \exp(-k_{21} \tau) & \phi_2^- & \phi_2^+ \exp(-k_{22} \tau) \\
\end{bmatrix} \begin{bmatrix}
G_{2,1} \\
G_{2,2} \\
G_{2,-1} \\
G_{2,-2} \\
\end{bmatrix} + \begin{bmatrix}
B \\
B \\
B \\
B \\
\end{bmatrix}.
\]

Note that \(\eta_{1/2}\) and \(\eta_{2/2}\) derived in Eqs. (21a) and (21b) are equivalent to \(B\). Once the four integration constants are solved from Eq. (34), we can compute the outgoing intensity parameters at the layer boundaries as follows:

\[
\begin{bmatrix}
I_1(\tau = 0) \\
I_{-1}(\tau = \tau_i) \\
I_2(\tau = 0) \\
I_{-2}(\tau = \tau_i) \\
\end{bmatrix} = \begin{bmatrix}
\Phi_1^+ & \Phi_1^- \exp(-k_{21} \tau) & \Phi_2^+ & \Phi_2^- \exp(-k_{22} \tau) \\
\Phi_1^- \exp(-k_{21} \tau) & \Phi_1^+ & \Phi_2^- \exp(-k_{22} \tau) & \Phi_2^+ \\
\phi_1^+ \exp(-k_{21} \tau) & \phi_1^- & \phi_2^+ \exp(-k_{22} \tau) & \phi_2^- \\
\phi_1^- \exp(-k_{21} \tau) & \phi_1^+ \exp(-k_{21} \tau) & \phi_2^- & \phi_2^+ \exp(-k_{22} \tau) \\
\end{bmatrix} \begin{bmatrix}
G_{2,1} \\
G_{2,2} \\
G_{2,-1} \\
G_{2,-2} \\
\end{bmatrix} + \begin{bmatrix}
B \\
B \\
B \\
B \\
\end{bmatrix}.
\]

Because \(I_1 = I_{-1}\) and \(I_2 = I_{-2}\) for a homogeneous layer, Eqs. (34) and (35) can be further reduced to the forms

\[
\begin{bmatrix}
0 \\
0 \\
\end{bmatrix} = \begin{bmatrix}
\Phi_1^+ \exp(-k_{21} \tau) + \Phi_1^- & \Phi_2^+ \exp(-k_{22} \tau) + \Phi_2^- \\
\phi_1^+ \exp(-k_{21} \tau) + \phi_1^- & \phi_2^+ \exp(-k_{22} \tau) + \phi_2^- \\
\end{bmatrix} \begin{bmatrix}
G_{2,1} \\
G_{2,2} \\
\end{bmatrix} + \begin{bmatrix}
B \\
B \\
\end{bmatrix}.
\]

Within the context of the four-stream approximation, we may carry out the delta-function adjustment for the phase function having a strong diffraction peak to achieve a higher accuracy in radiative transfer computation based on the similarity principle (Liou et al. 1988; Liou 2002). The optical depth, the single-scattering albedo, and the Legendre expansion coefficients of the phase function can be scaled according to the following equations:

\[
\tau' = (1 - f \sigma) \tau, \quad \sigma' = \frac{(1 - f) \sigma}{1 - \sigma f'},
\]

\[
\sigma_l = [\sigma_l - f(2l + 1)](1 - f), \quad \text{for } l = 0, 2, 3,
\]

where \(f\) is \(\sigma_0/9\). The similarity principle has been developed for the scalar intensity and its general applicability to the Stokes vector remains to be proven. However, it would be physically reasonable to apply the delta-function adjustment if the phase matrix elements exhibit strong forward peaks, similar to the phase function, to provide a better representation of the four-stream fitting.

Finally, since D4S only provides two upward and two downward radiative streams, we shall employ the integration technique to obtain the radiances in other directions for satellite application. The upward and downward Stokes vectors can be expressed as follows:
where the source function is given by

\[
I^+(0; \mu) = I^+(\tau_0; \mu) \exp(-\tau_0/\mu) \\
+ \int_0^{\tau_0} J(\tau'; \mu) \exp(-\tau'/\mu) \frac{d\tau'}{\mu},
\]

and

\[
I^-(\tau_0; -\mu) = I^-(0; -\mu) \exp(-\tau_0/\mu) \\
+ \int_0^{\tau_0} J(\tau'; -\mu) \exp(-(\tau_0 - \tau')/\mu) \frac{d\tau'}{\mu},
\]

where the source function is given by

\[
J(\tau, \mu) = \frac{\sigma}{2} \int_{-1}^{1} Z(\mu, \mu') I(\tau, \mu') d\mu' + (1 - \sigma) B[T(\tau)].
\]

On substituting the Stokes vector \( I_{sd}(\tau, \mu') \) computed from D4S into the \( I(\tau; \mu') \) term in the source function expression [Eq. (39c)], the Stokes vectors in Eqs. (39a) and (39b) can be determined at any satellite scanning angles. We then integrate the downward Stokes vector for each model layer progressively to the surface. Subsequently, we apply the surface reflection and emission boundary conditions to determine the upward Stokes vector from the surface. Finally, we integrate the upward Stokes vector for each model layer progressively to obtain the upward Stokes vector at the top of the atmosphere. These procedures can be accomplished efficiently in numerical computations.

4. Computational results and discussions

As an illustration of the accuracy and speed of D4S, we first show a comparison of the total solar spectral albedo (\( \lambda = 0.2 - 5 \mu m \)) at the top of the atmosphere computed from D4S and the exact method for an atmosphere containing a water cloud located between 0.83 and 2.75 km having a vertical optical depth of 10. The atmosphere extends from 0 to 50 km with a 1-km resolution. The exact method is based on the 16-stream doubling method to obtain the reflection and transmission for an atmospheric layer. Both methods employ the adding procedure to compute the spectral albedo in which the line-by-line equivalent radiative transfer model (Liou et al. 1998) uses the correlated \( k \)-distribution method for the sorting of absorption lines in the solar spectrum with a spectral resolution of 50 cm\(^{-1}\). The water cloud contains an effective radius of 8 \( \mu m \) and a midlatitude summer atmosphere with a surface albedo of 0.1 is used in the calculation along with two solar zenith angles of 30° and 75°. The D4S results are in excellent agreement with those computed from the exact method, as shown in Fig. 1. The mean relative differences are -0.192% and 0.682% and the root-mean-square differences are 0.00108 and 0.00377 for the two solar zenith angles, respectively. The required
CPU times for these results are 14.5 and 668 s in the SUN workstation Ultra 80 (a ratio of about 1 to 46) for D4S and the 16-stream doubling methods, respectively.

For illustration of the computational speed and accuracy involving thermal radiances, Fig. 2 shows comparison of the radiances at the discrete angles, $\mu_1 = 0.211325$ and $\mu_2 = 0.788675$, computed from D4S and a 40-stream doubling method (exact) for ice clouds having vertical optical depths between 0.01 and 10 with a mean effective ice crystal size of 24 $\mu$m for a thermal IR window frequency of 926 cm$^{-1}$ [one of the Atmospheric Infrared Sounder (AIRS) channels]. The single-scattering albedo in this case is 0.41099 and the asymmetry factor is 0.93973. Again, agreement is excellent with a mean relative difference of $-4.30 \times 10^{-5}$ (−0.25%) and a root-mean-square difference of 6.99 $\times$ $10^{-5}$ (0.4%). The required CPU time for these results are 0.01 and 0.61 s in the SUN workstation Ultra 80 (roughly at a ratio of 1 to 60) for D4S and the exact doubling method, respectively. Our doubling method was developed in Takano and Liou (1989a,b) and Liou and Takano (2002) for solar radiative transfer including polarization in which some computational results were checked with those listed in van de Hulst (1980). Subsequently, the doubling/adding program was extended to include polarized thermal emission, as presented in Takano and Liou (1993).

To check the accuracy and computational speed of the polarized D4S method outlined in section 3, we used a microwave frequency of 183 GHz [one of the channels in the Advanced Microwave Sounding Unit (AMSU)] and three ice cloud optical depths of 0.1, 1, and 10. Note that for thermal emission, Stokes parameters reach asymptotic values rapidly and the results for optical depths of 10 and 50 (as an example) are almost the same and will not be duplicated here. The ice cloud is composed of randomly oriented ice crystals with a maximum dimension of 300 $\mu$m and a width of 100 $\mu$m. The cloud temperature is 240 K corresponding to a Planck function of 7.268 $19 \times 10^{-5}$ [W m$^{-2}$ (cm$^{-1}$)$^{-1}$sr$^{-1}$]. The $2 \times 2$ phase matrix elements are approximated by a four-term Legendre polynomial expansion [$N = 3$ in Eq. (6)]. The two Stokes parameters computed from D4S are compared to those from the doubling method, which employs 40 streams (exact) in the calculation.

Figure 3 shows comparison of the phase matrix elements $P_{11}$, $-P_{12}/P_{11}$, $P_{22}/P_{11}$, and $P_{33}/P_{11}$ in the exact functional form and the two-term and four-term expansions in terms of the scattering angle. The exact phase matrix elements were computed using the finite-difference time domain method developed by Yang and Liou (2000). The element $P_{11}$ shows a peak at both forward and backward directions. The forward peak in this case is not sufficiently strong to require a delta-function adjustment. The angular distribution of $-P_{12}/P_{11}$ is opposite to that of $P_{11}$, with 0 at the forward and backward directions, but reaches a maximum value at the 90° scattering angle. The element $P_{22}$ has the same values as $P_{11}$ for all scattering angles. Finally, $P_{33}/P_{11}$ is positive in the forward direction, but negative in the backscattering direction. These four elements computed from the four-term expansion are almost identical to the exact values, as shown in Fig. 3. However, the two-term expansion results associated with the two-stream approximation significantly differ from the exact calculation. This comparison suffices to illustrate that using the 4-term expansion for the phase matrix elements is sufficiently accurate for microwave radiative transfer. In contrast, however, the two-term expansion for the phase matrix elements can produce large errors in radiance calculations.

Figure 4 illustrates comparison of $I$ and $Q$ Stoke parameters as functions of viewing zenith angle and cloud optical depth computed from D4S and the exact doubling method. The total radiance $I$ increases and de-
creases with increasing viewing zenith angle for thin ($\tau = 0.1$) and thick ($\tau = 10$) ice clouds, respectively. The radiances computed from D4S and the source function integration technique closely agree with those from the exact doubling method. The $Q$ parameter increases with increasing viewing zenith angle, reaching a peak between $60^\circ$ and $90^\circ$ for the three optical depths employed in the calculation. We see some deviation of the D4S approximation from the exact results, particularly for thin optical depth of 0.1 (about 10%). Note that the $Q$ parameter is associated with difference of the two radiance components and is a small quantity. If brightness temperature (directly converted from radiance via the Plank function) is used, however, differences become less than 4%. The two-stream method was found to produce large deviations from the exact calculations, and for small optical depths the $Q$ parameter displays unrealistic negative values. Calculations for other cases demonstrate that the D4S approximation can achieve an overall accuracy of within 5% for radiance and linear polarization (in terms of brightness temperature). Finally, we note that the computational speed for D4S is about 150 times faster than the exact doubling method.

5. Summary

In this paper, the fundamental equations governing the transfer of the Stokes vector in plane-parallel atmospheres for thermal emission are formulated and we show that the $[I, Q]$ component can be decoupled from the $[U, V]$ component. Subsequently, we develop the four-stream approximation for the transfer of polarized radiation in which the scattering phase matrix elements are expanded into four terms in association with the predetermined four radiative streams. Similar to the
scalar radiative transfer case, the solution of this approximation in vector form can be derived analytically so that an efficient computational method can be developed for radiance and polarization calculations. Moreover, by means of the source-function integration technique, the emergent radiation associated with satellite scanning angles other than the four-stream directions can be determined.

We provide a variety of illustrative cases to test the accuracy of D4S in comparison to the exact radiative

![Graphs showing the comparison of I and Q components as a function of viewing zenith angle computed from the D4S and the exact doubling method for a number of ice cloud optical depths.](image)

Fig. 4. Comparison of the I and Q components as a function of viewing zenith angle computed from the D4S and the exact doubling method for a number of ice cloud optical depths.
transfer calculations based on the doubling principle. We first compare the total solar spectral albedos (0.2–5 μm) computed from a line-by-line equivalent D4S and the exact method developed previously for an atmosphere containing a water cloud and show that differences between the two are less than 1%. Second, the D4S radiance calculations are shown to yield excellent accuracy for the transfer of thermal infrared radiation in the 10-μm window covering a spectrum of ice-cloud optical depths from 0.01 to 10. Third, employing the 183-GHz microwave frequency, we demonstrate that the four-term expansion of the four-phase matrix elements corresponding to the \([I, Q]\) Stokes component matches closely with the exact values, whereas the two-term expansion associated with the two-stream approximation produces significant deviations. Finally, we compare the \(I\) and \(Q\) values computed from the D4S polarized radiative transfer program developed in this paper to those from the exact doubling method using the 183-GHz frequency for an ice cloud containing large ice columns and plates. The radiances computed from the two methods match closely with differences less than 0.5% for all optical depths, while the polarization results show deviations of about 10% for thin optical depths from 0.01–0.1 because of small quantities. However, in terms of brightness temperature, the polarization deviation is less than 4%. Overall, in consideration of the computational speed and accuracy requirement the D4S approximation is shown to be the best solution for the simulation of infrared and microwave radiance and polarization for satellite data assimilation purposes.

**Acknowledgments.** This research has been supported by NOAA Grant NA03NES4400011 and in part by NSF Grants ATM-9907924 and ATM-0331550.

**APPENDIX A**

**Azimuthally Independent Expansion of Phase Matrix Elements**

The scattering phase matrix element \(Z_{ij}(\cos \theta)\) can be expanded in terms of Legendre polynomials in the form

\[
Z_{ij}(\cos \theta) = \sum_{l=0}^{N} (\bar{w}_{ij})_{l} P_{l}(\cos \theta), \quad \text{for } i, j = 1, 2, \tag{A1}
\]

where \(P_{l}(\cos \theta)\) is the Legendre polynomial of the \(l\)th order, and \((\bar{w}_{ij})_{l}\) is the expansion coefficient. Once the phase matrix elements are determined from the light-scattering theory, the value of \((\bar{w}_{ij})_{l}\) can be numerically determined based on the orthogonal property of Legendre polynomials. Using the addition theorem, we further expand \(Z_{ij}\) in terms of the spherical harmonic function as follows:

\[
Z_{ij}(\mu, \phi; \mu', \phi') = \sum_{m=0}^{N} \sum_{l=0}^{N} (\bar{w}_{ij})_{lm} P_{l}^{m}(\mu)P_{l}^{m}(\mu') \times \cos m(\phi - \phi'), \tag{A2}
\]

where

\[
(\bar{w}_{ij})_{lm} = (2 - \delta_{l0}m)(\bar{w}_{ij})_{l}(l - m)!, \quad \text{for } i, j = 1, 2. \tag{A3}
\]

Substituting Eq. (A2) into Eq. (5) in the main text, and performing azimuthal averaging, we obtain the expanded form of the azimuthally independent phase matrix elements in terms of the associated Legendre polynomials as follows:

\[
Z_{ij}(\mu, \mu') = \sum_{m=0}^{N} \sum_{l=0}^{N} (\bar{w}_{ij})_{lm} P_{l}^{m}(\mu)P_{l}^{m}(\mu'), \tag{A4}
\]

for \(i, j = 1, 2, \tag{A4}\)

where Eq. (A4) is identical to Eq. (6) in the main text. The expression for the coefficient \((\bar{w}_{ij})_{lm}^{m}\) differs for each phase matrix element and is given below.

The element \(Z_{11}\) is identical to the scattering phase function. It is independent of the azimuthal angle for thermal emission wavelengths so that

\[
Z_{11}(\mu, \mu') = \sum_{m=0}^{N} \sum_{l=0}^{N} \delta_{lm}(\bar{w}_{11})_{l} P_{l}^{m}(\mu)P_{l}^{m}(\mu') = \sum_{l=0}^{N} (\bar{w}_{11})_{l} P_{l}(\mu)P_{l}(\mu'). \tag{A5}
\]

According to Eq. (A5), \((\bar{w}_{11})_{l}^{m} = \delta_{lm}(\bar{w}_{11})_{l}\). The coefficient for the other three elements contains an azimuthal integration term. Thus

\[
(\bar{w}_{12})_{l}^{m} = (\bar{w}_{12})_{l}^{m} \times \frac{1}{2\pi} \int_{0}^{2\pi} \cos 2l_{1} \cos m(\phi - \phi') d\phi d\phi', \tag{A6}
\]

\[
(\bar{w}_{21})_{l}^{m} = (\bar{w}_{21})_{l}^{m} \times \frac{1}{2\pi} \int_{0}^{2\pi} \cos 2l_{2} \cos m(\phi - \phi') d\phi d\phi', \tag{A7}
\]
\[
(\mathbf{\omega}_{22})^m = (\mathbf{\omega}_{22})^m \\
\times \frac{1}{2\pi} \int_0^{2\pi} \cos^2 \phi \cos \phi' \sin \phi \cos \phi' \sin \phi' d\phi d\phi' \\
- (\mathbf{\omega}_{33})^m \\
\times \frac{1}{2\pi} \int_0^{2\pi} \sin^2 \phi \sin \phi' \cos \phi \sin \phi' \cos \phi' d\phi d\phi'.
\]

(A8)

The azimuthal integration terms in Eqs. (A6)–(A8) can be numerically evaluated by the Simpson rule.

APPENDIX B

Numerical Solution of the Characteristic Equation for Eigenvalues

Based on the similarity between Eq. (23) and the scalar quadratic equation, the following formula is supposed to be the solution

\[
k_i^2 = (a_i^2 \pm \sqrt{a_i^2 + 4b_i})/2, \quad j = 1, 2.
\]

(B1)

However, we are unable to obtain \( f(k) = 0 \) by substitution of Eq. (B1) into Eq. (23) because matrix multiplication is not commutable. As an alternative, the Newton–Raphson numerical method (Press et al. 1986) is used to obtain the solution for Eq. (23).

Let \( K^2 = K \), Eq. (23) can be rewritten as

\[
K^2 - aK - b = 0, \quad i = 1, 2.
\]

(B2)

Further, let \( K = [K_{ij}]_{2 \times 2}, \quad a_i = [(a_i)_{ij}]_{2 \times 2}, \quad \text{and} \quad b_i = [(b_i)_{ij}]_{2 \times 2} \), we can obtain four algebraic equations from Eq. (B2) for each \( i \) as follows:

\[
K_{11}^2 + K_{12}K_{21} - (a_i)_{11}K_{11} - (a_i)_{12}K_{21} - (b_i)_{11} = 0, \quad (B3)
\]

\[
K_{11}K_{12} + K_{12}K_{22} - (a_i)_{11}K_{12} - (a_i)_{12}K_{22} - (b_i)_{12} = 0, \quad (B4)
\]

\[
K_{21} + K_{22}K_{21} - (a_i)_{21}K_{21} - (a_i)_{22}K_{22} - (b_i)_{21} = 0, \quad (B5)
\]

\[
K_{22}^2 + K_{12}K_{21} - (a_i)_{22}K_{22} - (a_i)_{22}K_{22} - (b_i)_{22} = 0. \quad (B6)
\]

To apply the Newton–Raphson method, let \( K_i = x_i \) for \( n = 1–4 \), and let the left-hand side of Eqs. (B3)–(B6) be denoted as \( f_n(x_n) \) for \( m = 1–4 \), in which we approximate \( f_n(x_n) \) as the first-order truncated Taylor series expansion in the form

\[
f_n(x_n) = f_n(x_{n0}) + \sum_{m=1}^{4} \frac{df_n}{dx_n} |_{x_{n0}} (x_n - x_{n0}),
\]

for \( m = 1–4 \). (B7)

We may let the left-hand side of Eq. (B7) to be 0 to obtain a set of four simultaneous linear equations in \( x_n \)

\[
\sum_{m=1}^{4} \frac{df_m}{dx_n} |_{x_{n}} (x_m^{[p]} - x_m^{[p-1]}) = -f_m(x_m^{[p-1]}), \quad (B8)
\]

where the superscript \([p]\) denotes the iteration index. Using \( K_i \) obtained from Eq. (B1) as initial values for \( x_n \), we proceed to solve Eq. (B8) for \( x_n \) iteratively. The iteration stops when the following convergence criterion is satisfied:

\[
\sum_{m=1}^{4} |f_m(x_m^{[p]})| < 10^{-6} \quad \text{or} \quad |x_m^{[p]} - x_m^{[p-1]}| < 10^{-6}. \quad (B9)
\]

 Normally, five iterations are sufficient to achieve convergence.

REFERENCES


