Photon conservation in scattering by large ice crystals with the SASKTRAN radiative transfer model

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Abstract
The scattering of visible light by ice crystals and dust in radiative transfer models is challenging in part due to the large amount of scattering in the forward direction. We introduce a technique that ensures numerical conservation of photons in any radiative transfer model and that quantifies the integration error associated with highly asymmetric phase functions. When applied to a successive-orders of scatter model, the technique illustrates the high accuracy obtained in numerical integration of molecular and aerosol scattering. As well, a phase function truncation and renormalization technique is applied to scattering by ice crystals with very large size parameters, between 100 and 1000, and the scaled radiative transfer equation is solved with the spherical successive-orders model, SASKTRAN. Since computations shown this work are performed in a fully spherical model atmosphere, the computed radiances are not subject to the discontinuity at the horizon that is inherent in models using a plane–parallel assumption. The methods introduced in this work are of particular interest in modeling limb radiances in the presence of thin cirrus clouds.

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1. Introduction

Scattering of light by particles that are much larger than the wavelength typically displays an extremely sharp forward-scattering peak due to diffraction. This functional behavior of the scattering ‘phase function’ presents a significant challenge to radiative transfer models that rely on numerical quadrature of these functions to capture accurately the distribution of radiancy scattered by particles in the atmosphere.

Several approaches have been suggested for handling these highly forward-scattering phase functions in solutions of the radiative transfer equation. The majority of these methods have been focused on solutions by the discrete-ordinates family of models, where the distribution of zenith directions are prescribed by a Gauss quadrature rule. Within such a framework, sharp phase functions can be handled by modification to the Legendre-function expansion coefficients that form the basis for scattering operations. While this problem has reached some level of sophistication within the discrete ordinates model family, it continues to be an active problem within successive-order models and Monte Carlo models.

The majority of models that incorporate highly asymmetric phase functions belong to the discrete-ordinates family of models [1], which employ plane–parallel geometry. In such models, photon conservation is analytically guaranteed through the Gaussian quadrature by which the multiple-scattering ‘source’ term

$$J(\Omega') = k_{\text{scat}} \int 4\pi P(\Omega, \Omega') J(\Omega') d\Omega'$$  (1)
is computed, through the location of zeros in the interpolating polynomials. To obtain the directional volume emission rate $J$ in a direction $\Omega$, the radiance $I$ due to direct and diffuse contributions is integrated over all ‘incident’ directions $\Omega'$ and weighted by the angular probability of scattering, or phase function $P(\Omega, \Omega')$, and finally scaled by the single-scattering albedo $\omega = k_{\text{sc}}/k_{\text{ext}}$.

Since the handling of very strongly peaked phase functions within discrete-ordinates model requires the expansion of the phase function in increasingly high-order Legendre polynomials, the delta-Eddington [2] and delta-M [3] methods were introduced, which approximated the forward-scattering peak by a Dirac delta function, and thereby reduced the necessary number of expansion terms. The approximation of the forward-scattering peak by a delta function and truncation of the phase function was also done within a doubling-method model by Potter [4]. The oscillation errors introduced by the delta-M method were quantified by Nakajima and Tanaka [5], who also introduced a single-scattering correction to this method.

Iwabuchi and Suzuki [6] have implemented a geometric phase function truncation technique within a Monte-Carlo model, where polynomial expansions are not needed. This work introduced different approximations of the phase function that are used in each order of scatter.

While these methods are well-suited to their respective models, some inherent limitations limit their usefulness to some remote-sensing geometries. The plane-parallel geometry used by discrete-ordinate models results in a radiance discontinuity in the horizontal direction, which is quite prohibitive for use in limb-viewing remote sensing geometries. Little attention has been given to strong forward-scattering remote-sensing geometries. The plane–parallel geometry used by discrete-ordinate models results in a radiance discontinuity in the horizontal direction, which is quite prohibitive for use in limb-viewing remote sensing geometries. The plane–parallel geometry used by discrete-ordinate models results in a radiance discontinuity in the horizontal direction, which is quite prohibitive for use in limb-viewing remote sensing geometries.

In this paper we introduce an energy conservation technique that quantifies the accuracy of scattering computations in a successive-orders model. The technique illustrates the errors associated with the numerical scattering integral for several scattering particle types, from molecular Rayleigh scatter to particles with extremely sharply peaked phase functions. A phase function truncation and renormalization method is employed in a spherical successive-orders model, and is shown to reduce dramatically the errors associated with the source function evaluation. The energy conservation technique is used to analyze and select the truncation criteria to be used.

1.1. Equation of radiative transfer for scattered sunlight

In this work we are concerned with observations of scattered sunlight made in the atmospheric limb, so any radiance contributions from thermal emission are insignificant. In this case the equation of radiative transfer for the vector radiance $I$ in a direction $\Omega$ at position $r$ can be expressed as

$$\hat{\Omega} \cdot \nabla I(r, \Omega) = -n_0 K(r) I(r, \Omega) + n_0 \int_{4\pi} I(r, \Omega') Z(r, \Omega, \Omega') \, d\Omega'.$$

(2)

where $n_0$ is the number density of particles and $K(r)$ and $Z(r, \Omega, \Omega')$ are the extinction and scattering matrices, respectively. Since we are interested in modeling as applied to fast retrievals of atmospheric species with a radiative transfer model, we focus on unpolarized radiances, in which case Eq. (2) reduces to the equation for the scalar radiance $I(\Omega)$,

$$\hat{\Omega} \cdot \nabla I(\Omega) = -k_{\text{ext}}(\Omega) + k_{\text{sc}} \int_{4\pi} I(\Omega) P(\Omega, \Omega') \, d\Omega'. $$

(3)

Here $k_{\text{sc}}$ and $k_{\text{ext}}$ are the scattering and total extinctions, respectively, and the scattering phase function is denoted by $P(\Omega, \Omega')$. Further, we consider unpolarized radiances from scattering particles in a random orientation, and so the phase function can be expressed as $P(\Omega, \Omega') = P(\cos \theta)$, where the overbar in the scattering phase function denotes the weighted mean over all scattering particles. In this and all subsequent expressions the positional dependence of quantities in Eqs. (2) and (3) is assumed.

Since the observed radiance field, $I(\Omega)$, is heavily dependent on the particles composing the medium, the solution of the equation of transfer must take this into consideration. In the case of light scattering by particles that are very large compared with the wavelength, the large forward diffraction peak produces a phase function $P(\cos \theta)$ that is characterized by very strong forward-scattering behavior that increases together with size parameter.

1.2. Transport approximation

It has been shown [7] that the very sharply peaked nature of the phase function can be used as a simplifying assumption if $P$ is expressed as the sum of a sharply peaked component and a smoothly varying component, $P(\cos \theta) = P_s(\cos \theta) + P_t(\cos \theta)$. When substituted into the radiative transfer equation (3), one obtains

$$\hat{\Omega} \cdot \nabla I(\Omega) = -k_{\text{ext}}(\Omega) + k_{\text{sc}} \int_{4\pi} I(\Omega') P_s(\cos \theta) \, d\Omega', $$

(4)

where

$$k_{\text{ext}} = (1-\omega f) k_{\text{ext}}, \quad k_{\text{sc}} = (1-f) k_{\text{sc}},$$

and where

$$f = \int_{-1}^{1} P_s(\cos \theta) \, d(\cos \theta). $$

(5)

(6)

The fraction of incident light that scatters directly forward, $f$, is expressed through the normalization condition for phase functions, and in an unpolarized radiative transfer model, light that scatters according to $P_s(\cos \theta) = 2 \delta(1-\cos \theta)$ is effectively non-scattered light. From the phase function normalization condition, $\int_{4\pi} (P_s/4\pi) \, d\Omega = 1$, the normalization criterion for the smoothly varying component $P_t(\cos \theta)$ is

$$\int_{4\pi} P_t(\Omega, \Omega') \, d\Omega' = 1.$$

(7)

As shown by McKellar and Box [7], Eq. (4) is equivalent to the radiative transfer equation (3) modified by the scale transformations (5) and with the source term is computed
from the renormalized ‘smooth’ scattering component,
\[ j(\Omega) = \tilde{k}_{sc}(s) \int_{4\pi} I(\Omega') \tilde{P}_{\lambda}(\Omega, \Omega') \, d\Omega'. \]  
(8)

This scheme is often referred to as the transport approximation, and has been applied in a number of radiative transfer models [3].

1.3. Photon conservation diagnostic

The approximation described above is a powerful way to avoid numerical instabilities in the computation of the multiple-scattering source term, \( J \), for particles with highly asymmetric scattering. Unfortunately, the only information obtained in this method about the impact on computed radiances is the fraction of effectively unscattered light, \( f \). It is desirable to have quantitative information about the effects both of numerical integration errors and phase function truncation. If a photon conservation diagnostic criterion is used, these effects can be studied separately, and model configurations can be modified accordingly.

Within most radiative transfer models, the radiances incident to a given point are specified at discrete locations that can be denoted by a set of unit vectors, \( \Omega_j \), for \( j = 1 \ldots N_a \) where \( N_a \) is the number of incident discrete locations. Numerical conservation of photons within scattering operations can be investigated through the value of the scattered source function, \( j(\Omega, \Omega') \), that results from a single incoming radiance, \( I(\Omega) \). That is, we can consider the scattering of the radiance incoming at \( \Omega_j \) into all emerging directions \( \Omega' \) and integrate over all emerging radiance directions, \( \Omega' \). Then for ideal numerical photon conservation, it will hold that a dimensionless number \( \kappa(\Omega_j) \) will be equal to unity in the expression
\[ \kappa(\Omega_j) \cdot I(\Omega_j) \tilde{k}_{sc}(s) \Delta \Omega_j = \int_{4\pi} j(\Omega, \Omega') \, d\Omega. \]  
(9)

The numerical value \( \kappa(\Omega_j) \) is particular to that discrete location of incoming radiance, and indicates the accuracy of the scattering integral evaluation, Eq. (1). Any deviation of \( \kappa \) from unity indicates violation of conservation of energy in a numerical sense.

This conservation diagnostic technique can be applied to practically any radiative transfer model or observation geometry and is not restricted to any particular set of incident radiance directions, \( \Omega_j \). In what follows we describe its applicability to a successive-orders model in a spherical ray-tracing geometry.

2. The SASKTRAN model

The SASKTRAN radiative transfer model [8] employs a successive-orders solution within a fully spherical geometry that has been designed to model limb-scattered sunlight measured by the OSIRIS instrument [9] and can be fully configured to arbitrary viewing geometries. SASKTRAN is used operationally for retrievals of O₃ [10,11]; NO₂ [12]; and sulphate aerosols [13]. For example, to compute the modeled radiance for one simulated high-resolution OSIRIS scan (200 observer lines of sight that scan the limb) for one wavelength on a standard desktop computer takes approximately 15 s for 20 orders of scatter.

2.1. Treatment of scattering orders

Within SASKTRAN, all rays for the first two orders of scatter are traced exactly through a spherical model atmosphere. Ray-tracing shells with homogeneous scattering and absorption properties are configured at altitudes above a model spherical earth, whose radius is identified with the earth radius along the local meridian.

For higher orders of scatter, where the diffuse radiance is known to vary smoothly with solar zenith angle, the radiance field is computed at a set of ‘diffuse points’ specified by altitude and solar zenith angle coordinates. At each diffuse point, the previous-order radiance field is tabulated at ‘incoming’ directions \( \Omega_i \), which are distributed on the zenith–azimuth grid shown in Fig. 1. As illustrated in Fig. 1a, the incoming zenith directions are most densely located near the horizontal direction to capture the significant change in incoming radiance near the horizon. Since the angular separation of incoming zeniths is chosen to capture the variation in incoming radiance, it is widest in the upward-facing directions and slightly narrower in the ground-intersecting region.

2.2. Incoming and outbound ray distributions

At each diffuse point, previous-order radiance is scattered using Eq. (1) into a set of source terms, \( J \), specified at ‘outbound’ directions \( \Omega' \) by
\[ J_{i+1}(s, \Omega') = k_{sc}(s) \int_{4\pi} I_i(s, \Omega) \tilde{P}(s, \Omega, \Omega') \, d\Omega'. \]  
(10)

In this expression the order of scatter is indicated by the subscripts on \( J \) and \( I \). The outbound source functions are located at discrete directions \( \Omega_i \), specified by the minimum-energy distribution of Sloan and Womersley [14]. The location of points in this distribution constitute the minimum-energy configuration of a set of freely moving, equally valued point charges constrained to lie on the surface of a sphere.

The radiance modeled by SASKTRAN for any ray in the direction \( \Omega' \) is computed as
\[ I(s, \Omega) = I(s_1, \tilde{\Omega}) e^{-\tau(s_1, 0)} + \int_{s_1}^{s} I(s, \tilde{\Omega}) e^{-\tau(s, 0)} k(s) \, ds. \]  
(11)

The first term, the attenuated radiance of the ray end point, contains albedo-influenced terms from each order of scatter for rays that intersect the ground. The path integral in the second term evaluates the source functions (10) from all scattering orders by interpolating in height, solar zenith angle, and discrete outbound direction \( \Omega_k \). For the remainder of this paper, quantities \( I \) and \( J \) are assumed to occur at an optical depth \( \tau \) with path coordinate \( s \).

The incoming and outbound radiances for a diffuse point at 9.5 km altitude, together with the set of unit vectors at which they are specified, are shown on the unit sphere in Fig. 2. The azimuthal angles in these representations are measured with respect to the sunward direction, which is toward the left of the spheres. For the incoming radiances in Fig. 2a, as one moves from zenith
angles $\theta > 90^\circ$ through the horizon to $\theta < 90^\circ$, the incoming radiances move from contributions from the bright ground and very bright lower atmosphere to those from the very thin atmosphere above. In the outbound radiances in Fig. 2b, the broad and weak backward-scattering peak that results from Rayleigh scattering is visible.

The solid angle, $\Delta \Omega_j$, associated with each of the incoming directions shown in Fig. 2a can be interpreted as an equivalent cone of angular width $\Theta_i$, as illustrated in Fig. 3. For the distributions of points shown, the mean angular width of these cones is $\Theta_i \approx 3^\circ$, and for the ‘outbound’ points, the solid angle cone width is $\Theta_o \approx 6.4^\circ$. When the integral (10) is expressed numerically within SASKTRAN as a summation

$$J_{i+1}(\hat{\Omega}_k) \approx k_{sc} \sum_{j=1}^{N_{in}} I_i(\hat{\Omega}_j) \mathcal{P}(\hat{\Omega}_k, \hat{\Omega}_j) \Delta \Omega_j$$

over all incoming directions, $N_{in}$, where the incoming cone width is essentially the phase function sampling resolution. In the discretization of the multiple-scattering integral (1), directions $\hat{\Omega}$ are discretized into outbound directions $\hat{\Omega}_k$ with associated solid angle $\Delta \Omega_k$, and the same for incoming directions discretized into $\hat{\Omega}_j$.

It is implicit in the approximation of the integral (10) by the summation (12) that the value $\mathcal{P}(\hat{\Omega}_k, \hat{\Omega}_j)$ is the mean value of the phase function over the scattering
angles prescribed by the outbound direction, \( \hat{\Omega}_k \), and the set of all points within the incoming solid angle \( \Delta \Omega_j \). If the phase function is smoothly varying, then that mean value is well-represented by the value of the phase function at the central scattering angle, \( P(\hat{\Omega}_k \cdot \hat{\Omega}_j) \). In this case the summation becomes

\[
I_{j+1}(\hat{\Omega}) \approx k_{\text{scat}} \sum_{j=1}^{N_{\text{out}}} l_j(\hat{\Omega}_j) P(\hat{\Omega}_k \cdot \hat{\Omega}_j) \Delta \Omega_j. \tag{13}
\]

This approximation is subject to two assumptions. First, the incoming directions \( \hat{\Omega}_j \) must be sufficiently close that there is no significant change in the radiances \( I_j \) over its solid angle \( \Delta \Omega_j \). Second, the angular sampling of the ray distributions must be sufficient to capture the change of the phase function with scattering angle. Then if phase functions with extremely sharp features are used within the summation (13), one might expect that the outbound radiances are quite poorly behaved.

The primary operational use of SASKTRAN is as a forward model for retrieving atmospheric profiles of O\(_3\), NO\(_2\), and stratospheric aerosols, which have smoothly varying phase functions. It is shown in what follows that the approximation (13) is suitable for Rayleigh scattering and Mie scattering by stratospheric sulphate particles, but fails quickly as the forward-scattering probability increases with size parameter \( x \).

3. Method

3.1. Photon conservation in SASKTRAN

The photon conservation technique introduced in Section 1.3 can be applied to the SASKTRAN model by considering the set of incoming and outbound radiances directions, denoted here by \( \hat{\Omega}_j \) and \( \hat{\Omega}_k \), respectively. From Eq. (9), \( \kappa \) is expressed as

\[
\kappa(\hat{\Omega}_j) = \frac{\int_{\Omega_j} l_j(\hat{\Omega}_j) \, d\Omega}{k_{\text{scat}} \Delta \Omega_j}, \tag{14}
\]

and since the outbound directions \( \hat{\Omega}_k \) in SASKTRAN contain \( N_{\text{out}} \) spherical cubature weights \( w_k \), the conservation condition of Eq. (14) can be expressed as

\[
\kappa(\hat{\Omega}_j) = \frac{\sum_{k=1}^{N_{\text{out}}} w_k l_j(\hat{\Omega}_k, \hat{\Omega}_j)}{k_{\text{scat}} \Delta \Omega_j}. \tag{15}
\]

Because the incoming radiances is assumed constant over the solid angle \( \Delta \Omega_j \), Eq. (15) can be expressed simply using Eq. (12) in terms of the mean phase function over the incoming solid angle,

\[
\kappa(\hat{\Omega}_j) = \sum_{k=1}^{N_{\text{out}}} w_k P(\hat{\Omega}_k, \hat{\Omega}_j). \tag{16}
\]

and if the phase function is smoothly varying, the scaling factors evaluate to

\[
\kappa(\hat{\Omega}_j) = \sum_{k=1}^{N_{\text{out}}} w_k P(\hat{\Omega}_k \cdot \hat{\Omega}_j). \tag{17}
\]

For each scattering event in this work we compute the quantities \( \kappa(\hat{\Omega}_j) \) for each incoming direction using Eq. (17), and each outbound radiances is divided by the scaling factor \( \kappa(\hat{\Omega}_j) \) appropriate to each incoming direction. For scattering by particles with highly asymmetric phase functions, these factors depart significantly from unity, and the scaling of outbound radiances introduces a false re-distribution of radiances. This problem is addressed in Section 4.

The scaling factors \( \kappa \) constitute a set of values defined as a function of incoming direction \( \hat{\Omega}_j \) that evaluate to unity when the integral (10) is well approximated by the summation (13). The departure of these factors from unity is illustrated in Fig. 4 by modeling the scattering of 750 nm light by successively larger particles for a diffuse point at an altitude of 24.5 km. The scaling factors \( \kappa(\hat{\Omega}_j) \) are computed according to Eq. (17) and are specified at the incoming directions illustrated by the points in Fig. 1b. Note that the scaling factors displayed in this figure are shown on a logarithmic scale.

When a diffuse point is dominated by Rayleigh scattering as occurs with molecular-only scattering, the scaling factors evaluate to unity to eight decimal places of accuracy, as seen in Fig. 4a. The scaling factors for the same altitude, but when a sulphate aerosol layer is added to the molecular background, are shown in Fig. 4b. The aerosol scattering used in this computation assumes lognormally distributed particles of background size \( r_m = 0.08 \text{ nm}, s_m = 1.6, k_{\text{sca}} = 10^{-5} \text{ cm}^{-1} \). From the colorbar scale in this figure, it is seen that the phase function quadrature for scattering by stratospheric aerosol is accurate to four decimal places.

When slightly larger particles with a lesser degree of symmetry, such as subvisual cirrus ice crystals, are added to the molecular background atmosphere, a more significant departure from unity is seen. The scaling factors computed for T-matrix [15] simulated ice cylinders (aspect ratio of unity) in a gamma distribution with volume-effective mode radius \( r_c = 1.0 \text{ nm}, \) shape parameter 0.113, and number density \( n = 1 \text{ cm}^{-3} \) are shown in Fig. 4c. At this particle size, the inaccuracy in the phase function integration has become more significant, with accuracy now at two decimal places.

If particles with larger size parameters are involved in scattering, the scaling factors become very widely distributed, and the redistribution or ‘smearing’ effect involved in the scaling of radiances becomes very significant. The scattering properties from the in situ database of Baum et al. [16] are used in SASKTRAN to simulate scattering by cirrus clouds with a typical ice crystal size distribution and particle habit. This database contains scattering properties for a large variety of ice crystal habits that are based on in situ collection of cloud particles, with effective particle sizes ranging between 10 and 180 \( \mu \text{m} \). The tabulated phase functions are very sharply peaked in the forward direction, as can be seen in Fig. 5a in the following section.

As a worst-case example of numerical instability of the scattering integral, the values \( \kappa \) for scattering of 750 nm light by ice crystals with an effective size of \( D_e = 180 \mu \text{m} \) and number density \( 10^4 \text{ cm}^{-3} \) are shown in Fig. 5d. The inadequacy of the assumptions underlying the sum in Eq. (13) is clear from this figure. Radiance computations involving such scattering parameters are quickly divergent. The
The majority of incoming directions in this case have $\kappa < 1$ since the combinations of scattering angles specified by $\Omega'_k \cdot \Omega'_j$ do not sample the very narrow forward-scatter peak, and a few incoming directions have scattering angles sufficiently close to zero that their values $\kappa$ are over $10^2$. There is a thin band for zeniths near $180^\circ$ that has a value $\kappa$ near $3 \times 10^4$.

A small improvement to this situation results if the mean value of the phase function over the incoming solid angle $\Delta\Omega'_k$ is used instead of the value at $\Omega'_k \cdot \Omega'_j$. If a set of points is distributed on the incoming unit sphere at very high resolution in both zenith and azimuth, then the mean value of the phase function can be taken for all scattering angles between $\Omega'_k$ and each high-resolution point in $\Delta\Omega'_j$. This higher-resolution sampling of the phase function improves the quality of the numerical integration. Fig. 5 shows the scaling factors that result if a set of points separated by $0.05^\circ$ in zenith and azimuth are used. At this resolution, the technique typically brings the values of $\kappa$ to within an order of magnitude of unity for incoming directions except a narrow band about $\theta = 180^\circ$ that samples the strong forward peak. This incoming direction lies directly opposite an outbound direction positioned at $\theta = 0^\circ$.

If the diffuse incoming radiance is well-represented by the incoming point distribution, this method presents a reasonable approach to reduce slightly the error introduced by the assumption in Eq. (16). This technique may be necessary for some conditions, but its usefulness is limited due to its computationally intensive nature. The evaluation of the mean phase function at angular separation of $0.05^\circ$ requires distributing 26 million points on the surface of the unit sphere, and the required phase function interpolations slow the scattering computation by a factor of several thousand.

3.2. Delta-function technique

The scattering phase functions from the database of Baum et al. [16] display an extremely sharp forward-scattering peak, with half of the incident radiation being scattered into a cone of width less than approximately $1^\circ$. When these highly asymmetric phase functions are expressed as a function of 

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**Fig. 4.** Scaling factors $\kappa(\Omega'_j)$ as a function of incoming direction for (a) molecular, (b) molecular + aerosol (0.080 µm), (c) molecular + $T$-matrix ice (1.0 µm), (d) molecular + large ice (180 µm) scattering. Scaling factors are displayed on a logarithmic scale.
cos Θ in Fig. 6a, as they are typically represented in many radiative transfer models, the sharp forward-scattering peak increasingly resembles a Dirac delta function as the size parameter increases. In this plot, at scattering angles less than 5° (when cos Θ ≈ 1), the value of the phase function can change by more than six orders of magnitude. When the same phase functions are shown with scattering angle on a logarithmic scale, as in Fig. 6b, the large fraction of energy that increasingly scatters into the near-forward direction as x increases is more clearly seen. As discussed in Section 1.2, these very sharply peaked phase functions can be expressed as the sum of a sharply peaked component and a smoothly varying component, with the resulting scaled equation of radiative transfer, Eq. (4).

We implement this technique in SASKTRAN by truncating the phase function at a cutoff angle Θc and using a constant-valued extrapolant for angles Θ > Θc. When this truncation and renormalization technique is applied to the diffuse point whose scaling factors k were shown in Fig. 4d, the resulting scaling factors are seen in Fig. 7a to be significantly closer to unity. The phase function in this case has been truncated to a value of 10² for all angles less than 1.2°. The P̄ averaging technique described above can further be applied to the scaling factors computed after truncation. This results in a small improvement in the range of scaling factors, as shown in Fig. 7b.

4. Analysis

Key factors in the error analysis of the application of these techniques are the selection of an appropriate truncation method and a definition for what is a ‘good’ value for k, that is, one that sets an upper limit on the acceptable amount of ‘smearing’ of source radiances when divided by k. Since we are concerned in this work with very large size parameters, the following analysis will focus exclusively on phase functions from the database of Baum et al. [16] for UV–visible and NIR wavelengths.

4.1. Phase function truncation method

The phase function truncation scheme used in this analysis uses a ‘smooth’ phase function \( P_s(\Theta) \) defined by

\[
P_s(\Theta) = \begin{cases} P(\Theta_c), & \Theta \leq \Theta_c, \\ P(\Theta), & \Theta > \Theta_c. \end{cases}
\]

The selection of an appropriate truncation criterion thus amounts to finding the ‘cutoff’ angle \( \Theta_c \) that minimizes the defined error criterion.

Other functional forms for \( P_s(\Theta) \) in the peak region have been used in both others’ previous work and in the current work on this problem. Potter [4] used a power-law extrapolation in the narrow forward peak, which approximates well the functional form seen in Fig. 6b for scattering angles just above 1°. Iwabuchi and Suzuki [6] used a constant value \( P_0 \) out to an angle \( \Theta_c \) that together conserve
the first and second Legendre moments of the phase function. Since neither of these approaches is qualitatively different to the one presented, but only modifies the resulting fraction $f$, and since the phase function derivative $dP/d\cos \Theta$ does not appear in radiative transfer calculations, it is quite sufficient to use the piecewise-continuous truncated phase functions $P_i$ described above.

Analysis of the truncation methods used in a successive-orders model should consider the angular resolution of scattering used within the model. An angular width of 3° thus gives a reasonable upper bound on the width of the forward peak that can be truncated without distorting scattering into neighboring directions.

It should be noted that although one could naively increase the numerical accuracy of the summation in Eq. (13) by using a finer-resolution grid of incoming zeniths and azimuths, this would quickly become prohibitive since memory usage and computational time in SASKTRAN increases rapidly with the number of incoming directions, $N_{in}$. Geometries needed for ray-tracing and scattering computations are linked to the incoming rays, while outbound rays have little overhead to allow fast computations of many orders of scatter. Accordingly, the number of outbound directions $N_{out}$ can be increased without a significant increase in computational time or memory usage. It is shown that this gives a slight improvement in the resolution of phase function sampling.

When investigating the effectiveness of phase function truncation, useful indicators for the distribution of $\kappa$ values are

$$\bar{\kappa} = \exp \langle |\log \kappa_i| \rangle$$

and

$$\sigma_\kappa = \sqrt{\langle (|\log \kappa| - \log \bar{\kappa})^2 \rangle},$$

the absolute geometric mean and deviation of $\kappa$. The values of these two parameters for the scaling factors shown in Figs. 4 and 7 are listed in Table 1, with those computed for Rayleigh scattering included for comparison.

![Fig. 7](image.png)

Fig. 7. Scaling factors $\kappa(\Omega_i)$ for scattering by 180 \(\mu\)m ice crystals when (a) truncation only and (b) truncation and T technique are applied. High-resolution points are distributed by 0.05° in zenith and azimuth. Scaling factors are displayed on a linear scale.

If the phase function for scattering of 750 nm light by 180 \(\mu\)m particles is truncated below $\Theta_c = 2.0°$, then the scaling factors that were shown in Fig. 4d are distributed much more favorably, as shown in Fig. 8. From this figure it is quite clear that a truncation angle near 2° will result in quite acceptable values of $\kappa$. It should be noted that the fraction $f$ of incident light that is considered to have scattered directly forward in this configuration is significant—over two-thirds. The worst-case values of $\kappa$ have been reduced from over $10^5$ to 1.4, and the spread about $\kappa = 1$ is very small: $\sigma_\kappa = 0.0594$. These values were computed for outbound rays distributed in 169 directions. The effect of changing the number of outbound directions can now be studied.

The values of $\bar{\kappa}$ and $\sigma_\kappa$ that result from truncation at cutoff angles between 0.13° and 3°, and for varying numbers of outbound directions, are shown in Fig. 9. Both $\bar{\kappa}$ and $\sigma_\kappa$ drop significantly for cutoff angles $\Theta_c \geq 1°$, and larger cutoff angles will produce values of $\kappa$ that are quite close to unity, since $\bar{\kappa} \leq 1.1$ and $\sigma_\kappa \leq 0.15$.

While this selection of cutoff criteria ensures that the overall behavior of the scaling factors is favorable, it is necessary to consider also the exceptionally large and small scaling factors that remain after truncation has been applied. For treatment of these values, we consider the number of incoming directions that have large absolute values of the score $Z_\kappa = (\log \kappa - \log \bar{\kappa})/\sigma_\kappa$. The number of incoming directions that have values $|Z_\kappa| > 3$ are shown,

<table>
<thead>
<tr>
<th>Dominant scattering particles</th>
<th>$\bar{\kappa}$</th>
<th>$\sigma_\kappa$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rayleigh</td>
<td>1.000000037</td>
<td>$1.25 \times 10^{-9}$</td>
</tr>
<tr>
<td>Mie sulphate (0.08 (\mu)m)</td>
<td>1.00049</td>
<td>$3.61 \times 10^{-4}$</td>
</tr>
<tr>
<td>T-matrix ice (1 mm)</td>
<td>1.0213</td>
<td>0.0162</td>
</tr>
<tr>
<td>Database ice (180 (\mu)m) (do-nothing)</td>
<td>2.7385</td>
<td>0.2875</td>
</tr>
<tr>
<td>(truncated)</td>
<td>1.0654</td>
<td>0.0473</td>
</tr>
<tr>
<td>(truncated+T)</td>
<td>1.0452</td>
<td>0.0266</td>
</tr>
</tbody>
</table>

Table 1

Comparison of scaling factors for scattering of 750 nm light from several sources.
again as a function of cutoff angle and number of outbound directions, in Fig. 10.

All outbound ray distributions show a significant drop in the number of directions with $|z_k| > 3$ at angles between 1.5° and 2.0°. When outbound ray distributions with either 324 or 400 points are used, there are no directions that have scores $|z_k| > 3$. This result is a significant improvement in the distribution of scaling factors, $\kappa$. From these considerations, it appears that using a distribution of 324 outbound points with a cutoff angle of 2° gives the best distribution of scaling factors. The distribution is shown in Fig. 11a.

This selection of truncation angle and outbound ray distribution also works well for smaller particle sizes, as shown by the scaling factors for 60 μm scattering particles in Fig. 11b.

4.2. Uniformity of outbound radiances

The scaling factors $\kappa$ introduced in Eq. (9) assist models by numerically ensuring energy conservation to within the accuracy of the cubature weights of the outbound unit sphere. However, as with any normalization technique, this will introduce an amount of false scattering when the outbound radiances are divided by the scaling factors, $\kappa(\Omega_j)$. As a measure of the effect of truncation and
renormalization on computed radiances, it is instructive to consider an isotropic diffuse intensity field, which gives outbound radiances as

\[ J_k = \sum_{j=1}^{N_{\Omega_k}} \frac{P(\Omega_k, \Omega_j) \Delta \Omega_j}{k_j}. \]

The degree of nonuniformity of the outbound radiances for isotropic incoming radiances indicates the amount of false redistribution, or 'scaling' of radiances by scaling factors significantly far from unity.

To illustrate, consider the scaling factors shown in Fig. 4d, which were computed from the non-truncated phase function for scattering of 750 nm light by 180 μm ice crystals. If an isotropic incoming radiances field is scattered into every outbound direction, the set of outbound radiances that result in the absence of scaling or phase function truncation – for 180 μm particles is shown in Fig. 12a. Note that these values are shown on a logarithmic scale.

Clearly, when no phase function truncation is done, there are several 'hot spots' where extremely large outbound radiances result when the forward-scatter peak is sampled. The majority of outbound radiances do not sample this peak, and thus have systematically low outbound radiances. We quantify the change in the outbound radiances through distribution parameters \( J, s_J, a \), and \( z_J \) defined analogously to the parameters (18) and (19) for \( k \).

Outbound radiances that result from photon conservation without truncation are shown in Fig. 12b for the same particle size. With the application of the scaling factors \( k \), the outbound radiances are all within an order of magnitude of unity, with the magnitude of the 'hot spots' reduced significantly. The distribution is much more isotropic, with the geometric mean changing from \( J = 3.4682 \) to \( 1.1057 \) and the width changing from \( s_J = 1.3515 \) to \( 0.1416 \). The outbound radiances for phase function truncation without photon conservation are shown in Fig. 12c. Here the distribution is shifted very favorably, with \( J = 1.0672 \) and
Finally, the combined effects of truncation and photon conservation are shown in Fig. 12d. In this case, the distribution has been made increasingly isotropic, as indicated by the minimum value in the parameters $J$ and $\sigma_J$.

In terms of the distribution parameters, truncation best shifts $J$ toward unity, while photon conservation best reduces the number of directions with a large $|z|$ score while at the same time keeping the width, $\sigma_J$, small. The photon conservation operation eliminates spurious production or loss of photons, but will do so at the cost of redistributing the radiances into other directions. Truncation alone effectively removes the sharp forward peaks, but does so with a loss of information on scattering behavior. A combination of photon conservation and phase function truncation is seen to produce the best approximation to the scattering integral.

5. Conclusions

A technique has been introduced in this work that ensures photon conservation in any radiative transfer model. A set of scaling factors is applied to the scattered radiances that ensures numerical energy conservation through quantification of the scattering integral accuracy. This technique is applicable over a wide range of scattering particles, for size parameters much smaller than unity up to $10^4$ for UV–visible and NIR wavelengths.

In this work, we consider the application of this technique to a spherical successive-orders of scatter model, SASKTRAN. In its standard implementation for retrievals of trace gas number densities (ozone and nitrogen dioxide) with molecular scattering, energy is conserved to an accuracy of $10^{-4}$. For scattering by typical stratospheric sulphate aerosols, energy is conserved to an accuracy of $10^{-4}$, and to an accuracy of $10^{-2}$ for 1 µm ice particles. For scattering by ice crystals with effective size between 10 and 180 µm, this technique together with phase function truncation and renormalization conserves energy to an accuracy of $10^{-2}$. The accuracy in modeled radiances for large ice crystals is significantly improved, from errors of several orders of magnitude to now several percent.

Fig. 12. Outbound radiances for isotropic incoming radiances for ice crystals with (a) no correction, (b) truncation applied (at $2^\circ$) with no scaling, (c) scaling applied with no truncation, and (d) scaling and truncation applied.
The methods introduced in this work allow for computations of limb radiance spectra in the presence of large scattering particles. Radiances computed in this model are not subject to the horizontal radiance discontinuity that is inherent in plane-parallel models, and as such are highly useful for modeling remote sensing measurements when optically thin cirrus and dust layers are present.

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