Quasi-ballistic light scattering - analytical models versus Monte Carlo simulations

Ioan Turcu\textsuperscript{1} and Mikhail Kirillin\textsuperscript{2}

\begin{itemize}
\item \textsuperscript{1} National Institute for Research and Development of Isotopic and Molecular Technologies, 65-103 Donath, 400293 Cluj-Napoca, Romania
\item \textsuperscript{2} Institute of Applied Physics of the Russian Academy of Sciences, 603950 Nizhny Novgorod, Russia
\end{itemize}

Email: ioan.turcu@itim-cj.ro

Abstract. Approximate analytical solutions for the light scattering in a plan parallel geometry, where each scattering behaves according to a Henyey-Greenstein (HG) phase function, are presented and compared with Monte Carlo simulations. Analyzing each \textit{n}th order scattered flux, the obtained angular spreading is very well described also by a HG phase function. However, the total scattered flux deviates from the HG type dependence revealing the limits of the approximations.

1. Introduction
The migration of photons in different particulate media is generally described by the radiative transfer equation (RTE) \cite{1} that expresses the energetic balance between the incident, outgoing, absorbed, and scattered photons. Since in realistic cases there are very few available analytical solutions for the RTE equation \cite{2}, several numerical techniques have been developed. Among the most widely used numerical methods the statistical Monte Carlo (MC) techniques have become ubiquitous representing a stochastic realization of the RTE being able to approximate the exact solution for a given problem with any desired accuracy. Their main drawback is the need to simulate a large number of photon paths in order to reach a high accuracy level. There are many MC codes (capable to perform direct or inverse MC simulations) that have been developed in various fields of science and technology that deal with radiation transfer in turbid media \cite{3-7}. Recently the Photon Transport Simulator MC software has been used to obtain the directions of the successive orders, multiple scattered photons using one-term and two-term Henyey-Greenstein (HG) as single particle phase function \cite{8}.

In a far field experiment the scattering volume, as a whole, can be regarded as a “macroscopic particle” characterized by an effective scattering phase function which can be described analytically \cite{9-11}. The effective phase function (EPF) describing multiple scattering processes can be obtained by adding together the contributions for all scattering orders. The procedure has been applied using the HG single particle phase function. The accuracy of the approximate analytic solutions for the EPF obtained in the quasi-ballistic light scattering (QBLS) regime has been systematically assessed \cite{12}, the theoretical results being tested experimentally \cite{12} on a well known model: polystyrene spheres in suspension.
The main goal of the present paper is to evaluate the correctness of the EFP analytic solutions by comparing them with simulation data given by MC codes.

2. The quasi-ballistic scattering

2.1. The effective phase function

If the absorption is neglected, the QBLS can be understood as a steady state redistribution process attained by balancing the populations of photons indexed by the scattering order [10, 11]:

\[ \phi(\tau, \mu) = \phi_0(\tau, \mu) + \phi_s(\tau, \mu) = \sum_{n=1}^{\infty} \phi_n(\tau, \mu) \quad (1) \]

In equation (1) \( \phi_0 \) stands for the reduced incident flux, \( \phi_s \) for the scattered flux and \( \phi_1; \phi_2; \ldots; \phi_n; \ldots \) for the first, second and \( n \)th order scattered fluxes, respectively. The two variables are the optical thickness \( \tau \) and the cosine of the polar angle \( \mu = \cos(\theta) \).

In axially symmetric geometries the directional distribution of scattered photons is frequently described by the \( \mu \)-dependent single particle HG phase function:

\[ f_{\text{HG}}(\mu) = \frac{1}{4\pi} \left( \frac{1-g^2}{1-2g\mu+g^2} \right)^{1/2} = \frac{1}{2\pi} \sum_{l=0}^{\infty} \left( l + \frac{1}{2} \right) g^l P_l(\mu) \quad (2) \]

given by its expansion in terms of Legendre polynomials, where \( g = \langle \mu \rangle \) is the anisotropy parameter. The \( n \)th order scattered fluxes are obtained as products of two functions:

\[ \phi_n(\tau, \mu) = \frac{\tau^n}{n!} e^{-\tau} f_n^{(\text{HG})}(\mu) \quad (3) \]

where the functions \( f_n^{(\text{HG})}(\mu) \) are the \( n \)th order phase functions describing the angular spreading of the corresponding scattered flux:

\[ f_n^{(\text{HG})}(\mu) = \sum_{l=0}^{n} \left( l + \frac{1}{2} \right) g^l P_l(\mu) = \frac{1}{2} \left( 1 - 2g^n \mu + g^{2n} \right)^{1/2} \quad (4) \]

The angular flux of scattered photons can be rewritten in a more compact form:

\[ \phi_s(\tau, \mu) = (1-e^{-\tau}) f_{\text{eff}}(\tau, \mu) \quad (5) \]

using the EPF \( f_{\text{eff}}(\tau, \mu) \) which can be given explicitly by [9, 11]:

\[ f_{\text{eff}}^{\text{HG}}(\tau, \mu, g) = \sum_{n=1}^{\infty} \frac{\tau^n}{n!} e^{-\tau} f_n^{(\text{HG})}(\mu) = \sum_{l=0}^{\infty} \left( l + \frac{1}{2} \right) \frac{(e^{\tau g}-1)}{e^{\mu \tau} - 1} P_l(\mu) \quad (6) \]

together with the \( \tau \)-dependence of the effective anisotropy parameter.

Unfortunately, although each \( f_n(\mu, g) \) may be expressed as HG type phase function, the coefficients in equation (6) don’t have the usual power type dependence in the polynomial order \( l \) which is characteristic for a HG phase function. To express the EPF as HG type phase function, the coefficients in equation (9) have been approximated by power type dependencies [10]:

\[ \frac{e^{\tau g}-1}{e^{\mu \tau} - 1} = g^{G(\tau)} \quad ; \quad G(\tau) = \frac{(\tau-1)e^{\tau} + 1}{(e^{\tau} - 1)} \quad (7) \]

As a direct consequence, the EPF can be also approximated by a HG phase function:
and by a fairly accurate expression of the anisotropy parameter.

2.2. Monte Carlo simulation

The Monte Carlo method applied to light propagation in scattering media is based on the calculation of trajectories of a large number of photons ($5 \times 10^7$ in our simulations) randomly migrating in a particulate medium (a suspension containing red blood cells in our case). The main hypothesis was that the single scattering event is suitably described by a HG phase function. The simulations were performed using a previously developed Monte Carlo algorithm [7, 14, 15], a 1 mm thick plan-parallel cuvette, and a haematocrit $H$ varying between $10^{-4}$ ($\tau = 0.076$) and $10^{-2}$ ($\tau = 7.6$). The upper limit of the $H$ values has been fixed low enough to maintain the relatively strong anisotropy of the scattering process. The red blood cells and the surrounding medium are supposed to be non-absorbing. The basic input parameters for MC simulations are the optical properties of the medium: the scattering coefficients of $\mu_s = 760 \cdot H$ [mm$^{-1}$] (for photons with $\lambda = 633$ nm), the single scattering anisotropy factor $g = 0.789$ and the used HG type phase function. The output parameters are the angular polar distributions (with a resolution of 0.05 degrees) of the photons scattered $n$ times considering the scattering process as axially symmetric.

3. Results

Monte Carlo simulation of scattered photons using a HG single scattering phase function showed good correlation with the theoretical predictions. Representative results are shown in figure 1 where the two types of MC simulations are presented: the angular spreading of the scattered photons (left side) and the $\tau$ -dependence of the number of photons scattered $n$ times (right side). The angular spreading of each scattering order is very well described by HG phase functions and the obtained anisotropies are very close to the predicted values, as can be observed in figure 3.a. Deviations from the theoretical predictions appear in the case of samples with higher optical thickness and/or for higher scattering orders. The corresponding errors are shown in figure 2. (the theoretical fluxes are given by equation(3))
Figure 2. The accuracy of the analytical model assessed by MC simulations. a) The \( \tau \)-dependence of the normalized fluxes of scattered photons. We show the analytic results obtained according to equation (3) together with the corresponding MC simulated values for the first 4 scattering orders. b) The flux relative error \( \varepsilon_{\text{rel}} = (\phi_a - \phi_{\text{MC}})/\phi_{\text{MC}} \) describing quantitatively the discrepancies between the theoretical predictions and the data obtained by MC simulations.

Figure 3b presents the decrease of the anisotropy parameter with the increase of the sample optical thickness. One can see from the beginning that there are differences between the two analytic functions \( g_a(\tau) \), \( g_{\text{MC}}(\tau) \) and also that the values obtained by MC simulations are systematically higher as compared to the predicted ones. The differences are reasonably small for optical thicknesses smaller than 1 but after that become more pronounced increasing with the increase of \( \tau \).

Figure 3. The assessment of the accuracy of the theoretical predictions concerning the anisotropy of the scattering process. a) The \( n \)th order anisotropy (for \( 1 < n < 6 \)) obtained by fitting the angular spreading of MC scattered photons is almost independent on the optical thickness of the sample. The obtained values are also very close to the theoretical predictions (dashed lines). b) The \( \tau \)-dependence of the predicted decrease of the scattering anisotropy. The MC simulations \( g_{\text{MC}}(\tau) \) are compared with the two theoretically obtained formula \( g_a \) and \( g_{\text{HG}} \).

4. Conclusions
The angular spreading of photons is very well described by HG type phase functions even for scattering orders larger than 10. The scattering anisotropy is also given by values that are very close to
theoretical predictions and even more are almost unaffected by the increase of the optical depth (see figure 3a).

On the other hand the MC simulated values of the photon fluxes corresponding to different scattering orders are smaller compared to theoretical predictions. The relative errors become significant by the increase of the optical depth and/or by the increase of the scattering order. The overall effect refers to a super-estimation of the contribution of the multiple scattered photons introduced artificially in the theoretical approach. The errors introduced by the used approximations are transferred in the corresponding unreasonable fast decrease of the anisotropy functions $g_{\alpha}(\tau)$, $g_{\mu \sigma}(\tau)$ compared to the corresponding values obtained by the MC simulations.

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