Implementation of polarization into a 3D Monte Carlo Radiative Transfer Model

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Abstract

Non-spherical particles scatter and polarize solar radiation depending on their shape, size, chemical composition and orientation. In addition, such information is crucial in radiative transfer modeling. Therefore, in this study, the implementation of polarization into a three-dimensional radiative transfer model is introduced and its validation through benchmark results. The model is based on the statistical Monte Carlo method (in the forward scheme) and takes into account multiple scattering and the polarization states of the monochromatic radiation. It calculates column-response pixel-based polarized radiative densities for 3D inhomogeneous cloudy atmospheres and is hence best suited for use in remote sensing applications. To this end, the model can be used to explore the potential of remote sensing techniques which distinguish between spherical and non-spherical particles on the one side and coarse mode dust particles and ice particles on the other side.

Zusammenfassung

Nichtsphärische Partikel streuen und polarisieren die solare Strahlung in Abhängigkeit ihrer Form, chemischen Zusammensetzung sowie Orientierung. Diese Informationen sind zudem auch entscheidend für Strahlungstransportmodelle. Deshalb wird in dieser Studie die Integration der Polarisation in ein dreidimensionales Strahlungstransportmodel vorgestellt und anhand von Bezugswerten validiert. Das Model basiert auf einer statistischen Monte Carlo Methode (Vorwärtsrechnungen) und beachtet zudem die Mehrfachstreuprozesse sowie den Polarisationsstatus der monochromatischen Strahlung. Es berechnet säulenweise und pixelbasiert polarisierte Strahldichten einer dreidimensionalen inhomogenen wolkigen Atmosphäre und ist somit bestens für Anwendungen im Fernerkundungsbereich geeignet. Abschließend ist dieses Model dazu geeignet, das Potential von Fernerkundungstechniken zu erkennen, die zur Unterscheidung von sphärischen und nichtsphärischen Partikeln sowie groben Staubpartikeln und Eiskristallen entwickelt wurden.

1. Introduction

Non-spherical particles are known to have a considerable impact on climate (Liou 1986; Kaufman et al., 2002; IPCC, 2007). They scatter and change the polarization state of solar radiation depending on their shape, size, chemical composition and orientation. Even though this relationship is rather complex, its knowledge is the prior condition for the interpretation of remote-sensing measurements. Additionally, the comprehensive investigation of ground-based and airborne-based passive radiometric and polarized measurements require a vector radiative transfer model that accounts for multiple scattering and polarization. Thus, in the present study, we introduce a new polarized model based on the forward Monte Carlo method that exactly simulates 3D radiative transfer processes in arbitrary complex scattering and absorbing media (i.e. clouds). Validations of the code against different benchmark results are also presented.

2. Methodology

The three-dimensional (3D) radiative transfer model at the Institute for Marine Research at the University of Kiel (UNIK) is the scalar model used for the purpose of this study (Macke, 1994). The model is based on the statistical forward Monte Carlo method and its main purpose is to calculate column-response pixel-based radiative densities for 3D inhomogeneous cloudy atmospheres. For this study, the model has been extended to take into account the polarization state of the monochromatic radiation due to multiple scattering by randomly oriented non-spherical particles, i.e. coarse mode dust particles and ice particles.

2.1. Model description

Following the comprehensive description by Cashwell and Everett (1959), the original scalar MC-UNIK model is considered to be a 3D Cartesian domain with a cellular structure, in which individual photons are traced until they either leave the scattering domain or are fully absorbed.

The 3D domain is divided into grid-boxes with indices (i, j, k) and geometrical dimensions along x-, y-, and z-direction. Each grid-box is characterized by a volume extinction coefficient $\beta(i, j, k)$ a scattering phase function $P(\Theta, I, j, k)$ with scattering angle Θ, and a single scattering albedo ω_o (see Fig. 1).

Directions are specified by means of an azimuth and zenith angle. The azimuth angle φ is measured clockwise when looking upwards and the zenith angle θ is the angle with respect to the downward normal. Additionally, free path lengths and scattering directions are simulated as outlined in Marchuk et al., (1980) by random number processes with Lamberts law of attenuation and the scattering phase function as the probability density functions for the free path length and the scattering direction.

Simulation begins with a photon entering randomly on the top layer (i, j, k_{max}) of the model domain. Each photon is characterized by a weight, whose value is set initially to unity. Its position is uniformly distributed with a propagation specified by the solar zenithal and azimuth angle (θ_o, φ_o) and direction described by the direction cosines:

$$k_{in}^{x} = sin\,\theta_o\, cos\,\varphi_o$$

$$k_{in}^{y} = sin\,\theta_o\, sin\,\varphi_o \qquad (1)$$

$$k_{in}^{z} = cos\,\theta_o$$

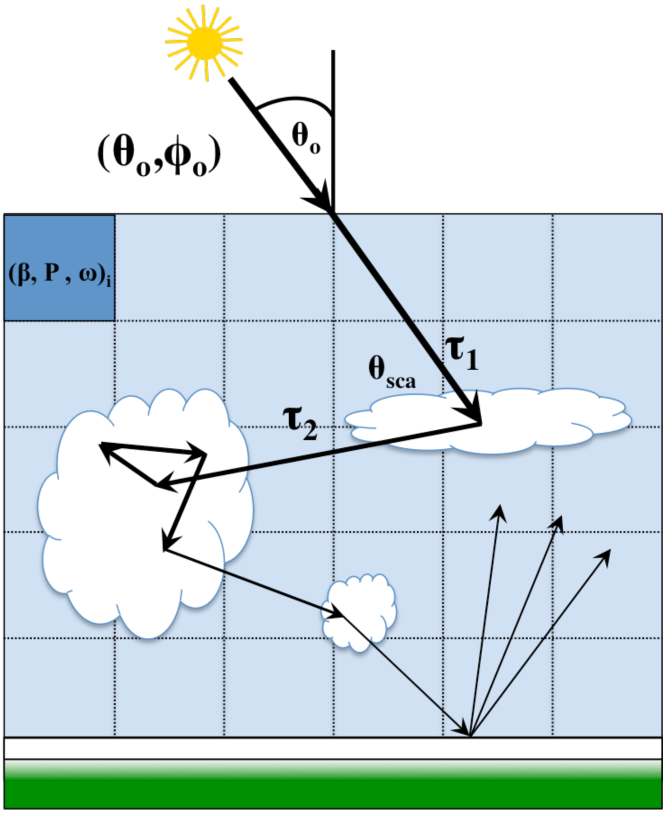

Fig. 1: Scheme of photon path within the 3D domain of the Monte Carlo radiative transfer model.

Photons are traced from the starting point on one grid-box surface to the intersection with the nearest neighbour grid-box surface as illustrated in Fig. 2, as described in Macke et al. (1999). This procedure is repeated l times until the cumulated optical thickness

$$\tau_{cum} = \sum_l \beta\,(i,j,k) t_l, \qquad (2)$$

exceeds the randomly chosen (exponentially distributed) optical thickness τ_{rand}. t_l stands for the step lengths within the individual grid-boxes. Subsequently, the photon steps backward by

$$t_{back} = (\tau_{cum} - \tau_{rand})/\beta(i,j,k), \qquad (3)$$

to ensure that the total photon path exactly matches the τ_{rand}.

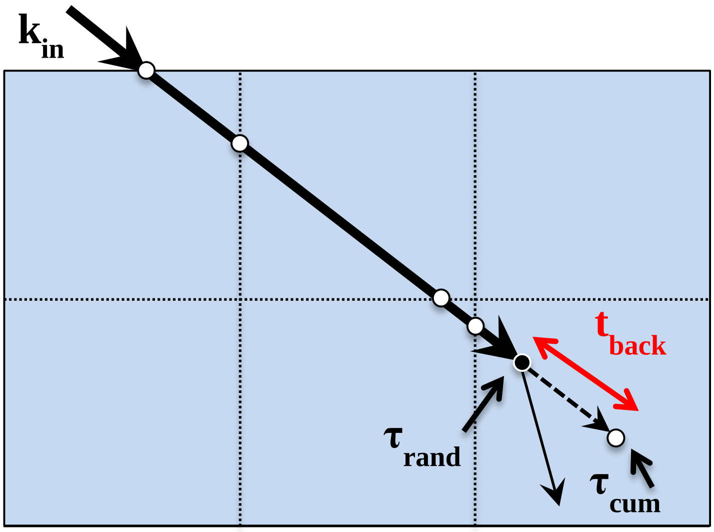

Fig. 2: Illustration of photon tracing within a regular array of cloud boxes.

The MC radiative transfer model directly simulates the scattering events. After travelling a certain path inside the domain a scattering event takes place and the new direction of the photon $k_{out} = (k_x, k_y, k_z)_{out}$ is calculated by the preceding direction and the scattering zenith and azimuth angles described in Marchuk et al. (1980), Chapter 2.2. In the scalar scheme, the scattering azimuth angle is uniformly distributed between [0, 2π] and the scattering zenith angle is randomly chosen from the precalculated cumulative probability density function according to

$$S_{i-1} < R < S_i \text{ with } S_i = \sum_{j=1}^{i} P\left(\theta_j\right)\Delta\Omega\left(\theta_j\right) \qquad (4)$$

Where $\Delta\Omega\left(\theta_j\right)$ is the solid angle interval corresponding to a finite scattering angle interval $[\theta_{i,min}, \theta_{i,max}]$ and R stands for a random number uniformly distributed between 0 and 1. The exact scattering angle is then interpolated by

$$\theta = \theta_{i,min} + t \cdot \theta_{i,max} \text{ with } t = \frac{R - S_{i-1}}{S_i - S_{i-1}}. \qquad (5)$$

In addition, absorption is taken into account by multiplying the initial photon weight by the single scattering albedo, whenever a scattering event occurs, and the surface contribution is calculated assuming a Lambertian surface (isotropic reflection).

In order to grant precise radiance calculations for each wavelength the so-called Local Estimate Method (LEM) has been applied (Collins et al., 1972; Marchuk et al., 1980; Marshak et al., 2005). The LEM accounts the probability that the photon is scattered into the direction of the sensor at each scattering process. It also calculates the attenuation along the optical thickness (τ) between the scattering location and the detector. It is described by:

$$w = \omega_o P\left(\theta_{inc,det}\right) \frac{\exp(-\tau)}{cos\theta_{det}}. \qquad (6)$$

Where $\theta_{inc,det}$ is the scattering angle between the incident direction and the direction of the detector, θ_{det} is the zenithal angle of the detector, and ω_o is the single scattering albedo. The division by $cos\theta_{det}$ is to account for the slant area in the radiance definition.

Finally, when the simulation ends, the normalized radiance is computed by:

$$I = \pi \frac{E(i,j)}{\mu_o F_o}, \tag{7}$$

where $\mu_o F_o$ is the incoming solar flux and E the radiance. The statistical errors of the fluxes and radiances are given by $1/\sqrt{n}$, where n is the number of photons (Macke et al. 1999).

2.2. Polarized Monte Carlo model

The conventional approach to handle polarization dates back to Sir George Gabriel Stokes. In 1952, he discovered that the polarization behaviour of the electromagnetic wave could be represented by real observables. This resulted in the Stokes vector, defined by four quantities $S = (I, Q, U, V)$, each of them carrying the units of irradiance (W/m^2) (Stokes, 1852). The latter allows the Stokes vector to describe the intensity and the state of polarization and it can be simply included to the radiative transfer theory.

The Stokes parameters are defined by the components of the electromagnetic field (e.g. Chandrasekhar, 1960; van de Hulst, 1957; Hansen and Travis, 1974; Liou, 2002; Mishchenko et al., 2002):

$$I = E_l E_l^* + E_r E_r^*, \tag{8}$$
$$Q = E_l E_l^* - E_r E_r^*, \tag{9}$$
$$U = E_l E_r^* + E_r E_l^*, \tag{10}$$
$$V = i(E_l E_r^* - E_r E_l^*). \tag{11}$$

Where E_l and E_r are two orthogonal electric field components parallel and perpendicular to the direction of propagation respectively, the asterisk stands for the conjugate value, and $i = \sqrt{-1}$. The first component of the Stokes vector, *I*, gives the total irradiance, Q and U describe the linear polarization and the circular polarization is given by *V*. Furthermore, the Stokes parameters are defined such that the local meridian plane acts as a plane of reference (Chandrasekhar, 1960) defined by the propagation direction (i.e. incident and scattered) of the photon and the vertical direction – *z*-axis.

In the following, we present the implementation of polarization in the MC model. To begin with, in the vector approach the scalar weight is replaced by the Stokes weight. The incident photon is supposed to be initially unpolarized and the corresponding weight is $S = (1,0,0,0)$.

Another important difference in the vector scheme concerns modifications in the scattering description. For many scattering problems (i.e. scalar radiative transfer theory, and randomly oriented particles), the phase function P, which represents the relative angular distribution of the scattered direction (Wendisch et al., 2012), is sufficient to describe thoroughly the scattering behaviour dependent only on the scattering angle with respect to the incident direction. However, polarization introduces an anisotropy on the scattering direction since it depends on the frame of reference. The scattering geometry is illustrated in Fig 3. For polarization problems (anisotropic scattering), the interaction between a photon and a particle is described by a 4x4 matrix, the so-called phase matrix. Considering an ensemble of randomly oriented particles the number of matrix elements could be reduced to six (van de Hulst, 1980):

$$P(\Theta) = \begin{pmatrix} P_{11}(\Theta) & P_{12}(\Theta) & 0 & 0 \\ P_{12}(\Theta) & P_{22}(\Theta) & 0 & 0 \\ 0 & 0 & P_{33}(\Theta) & P_{34}(\Theta) \\ 0 & 0 & -P_{34}(\Theta) & P_{44}(\Theta) \end{pmatrix}, \tag{12}$$

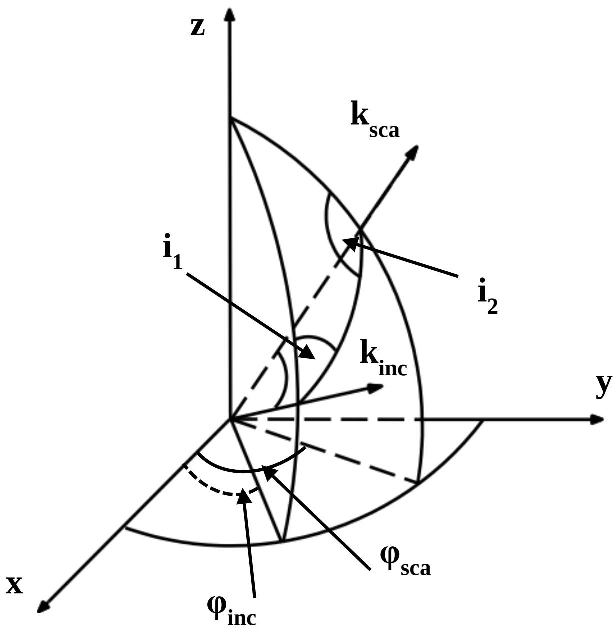

Fig. 3: The geometry of anisotropic scattering: incident k_{inc} and scattered k_{sca} directions. i_1 and i_2 are the rotation angles, and φ_{inc} and φ_{sca} are the azimuth angles of the incident and scattered directions respectively (Mishchenko et al., 2002).

The latter is defined with respect to the scattering plane, determined by the incident and the scattering directions. In addition, it relates the Stokes parameters linked to the two directions, specified with respect to their reference planes (Mishchenko et al., 2002). Hence, in order to derive the scattered Stokes vector $S_{sca} = (I, Q, U, V)_{sca}$ with respect to its plane of reference (plane containing the scattered and the vertical direction) one has to transform the incident Stokes vector $S_{inc} = (I, Q, U, V)_{inc}$ to the scattering plane so that the phase matrix multiplication can be carried out. Finally, the scattered Stokes vector is given by:

$$S_{sca} = R(\pi - i_2)P(\Theta)R(-i_1)S_{inc} = Z(\theta_{inc}, \varphi_{inc}, \theta_{sca}, \varphi_{sca})S_{inc}, \tag{13}$$

where Z is the transformation matrix that describes the scattering procedure, i_1 and i_2 are the rotation angles, the subscripts inc and sca stands for the incident $k_{inc} = (\theta_{inc}, \varphi_{inc})$ and the scattered directions $k_{sca} = (\theta_{sca}, \varphi_{sca})$ and $R(i)$ is the rotation matrix:

$$R(\mathrm{i}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos 2i & \sin 2i & 0 \\ 0 & -\sin 2i & \cos 2i & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{14}$$

The rotation angles can be computed from k_{inc} and k_{sca} using spherical trigonometry (Mishchenko et al., 2002):

$$\cos i_1 = \frac{\cos\theta_{sca} - \cos\theta_{inc} cos\Theta}{\pm\sin\theta_{inc}\, sin\Theta} \tag{15}$$

$$\cos i_2 = \frac{\cos\theta_{inc} - \cos\theta_{sca} cos\Theta}{\pm\sin\theta_{sca}\, sin\Theta} \tag{16}$$

$$\cos 2i_{1,2} = 2\cos^2 i_{1,2} - 1 \tag{17}$$

$$\sin 2i_{1,2} = 2\,(1 - \cos^2 i_{1,2})^{1/2} \cos i_{1,2} \tag{18}$$

The sign $\pm$ depends on the difference ($\varphi_{sca} - \varphi_{inc}$), and one should take limits when the dominator of the above equations becomes zero.

As we already mentioned, for polarization problems, the transformation matrix and not just the phase function describes the scattering behaviour. However, we use the phase function as the probability density function to obtain the scattering angle Θ and a randomly chosen angle (between 0 and 2π) to derive the scattering azimuth angle. We could let this happen by applying the following correction:

$$S_{sca} = P_{11}^{-1}\, Z\, S_{inc}, \tag{19}$$

In other words, in a case of scattering event we can sample Θ from the phase function, but we need to replace the transformation matrix Z with a reduced matrix $P_{11}^{-1} \cdot Z$. This method is called biased-sampling method or importance sampling method. For further information about this method the reader is referred to the literature (Collins et al. 1972; Kattawar, 1978; Marchuk et al. 1980).

3. Model validation

Benchmark results have been provided by plenty comparisons including Coulson et al. (1960), Garcia and Siewert (1986, 1989), Mishchenko (1991), de Haan et al. (1987), Natraj et al. (2009) among others. However, in this study we validate our polarized Monte Carlo radiative transfer model through Kokhanovsky et al. (2010) and Wauben and Hovenier (1992).

For a Rayleigh and aerosol layer we compared our model through Kokhanovsky et al. (2010). The benchmark results have been generated using SCIATRAN (Rozanov et al., 2005, 2006) which is a software package based on the discrete ordinates method.

Simulations were conducted for a homogeneous plane-parallel layer assuming a cloud optical thickness of 0.3262, a single scattering albedo of 1, and a black underlying surface (the surface albedo equals to 0, i.e. ideal absorbing) for both cases.

The Rayleigh phase matrix was given without the depolarization factor as in Eq. (20), and the aerosol phase matrix was calculated using Mie theory (Mie, 1908) at λ=412 nm. The phase matrices are shown in Fig. 4.

$$P_R(\Theta) = \frac{3}{4}\begin{pmatrix} 1+cos^2\Theta & cos^2\Theta-1 & 0 & 0 \\ cos^2\Theta-1 & 1+cos^2\Theta & 0 & 0 \\ 0 & 0 & 2cos\Theta & 0 \\ 0 & 0 & 0 & 2cos\Theta \end{pmatrix}, \tag{20}$$

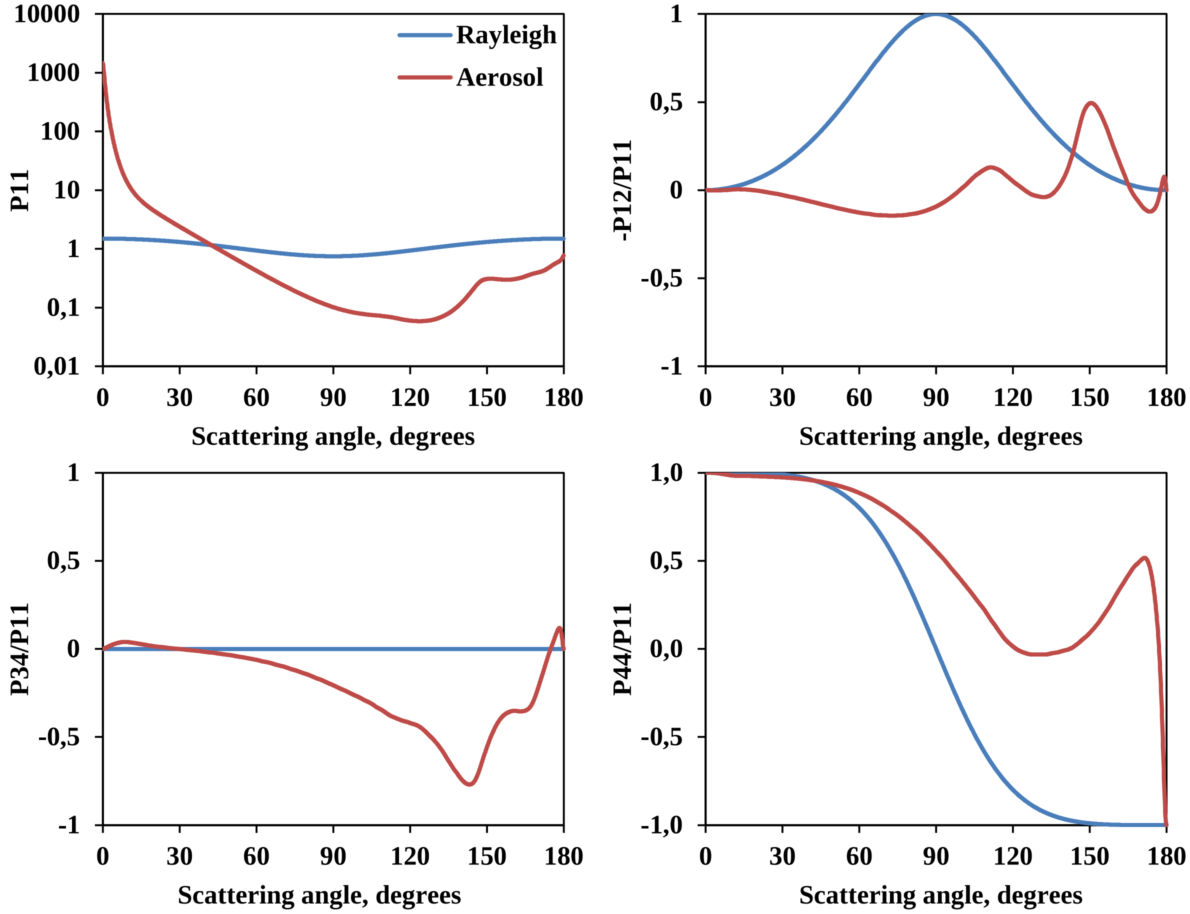

Fig. 4: Phase matrix elements for the aerosol case and for the Rayleigh scattering.

In Fig. 5 we present the normalized Stokes vector for the transmitted, $S_T=(I_T, Q_T, U_T, V_T)$, and reflected, $S_R=(I_R, Q_R, U_R, V_R)$, diffuse radiation pertaining to a solar zenith angle of 60°, relative azimuth angles between radiance and incident directions (RRA) of 0°, 90° and 180° and different view zenith angles (VZA). Note here that a relative azimuth angle of RRA = 0° corresponds to the exact backward scattering.

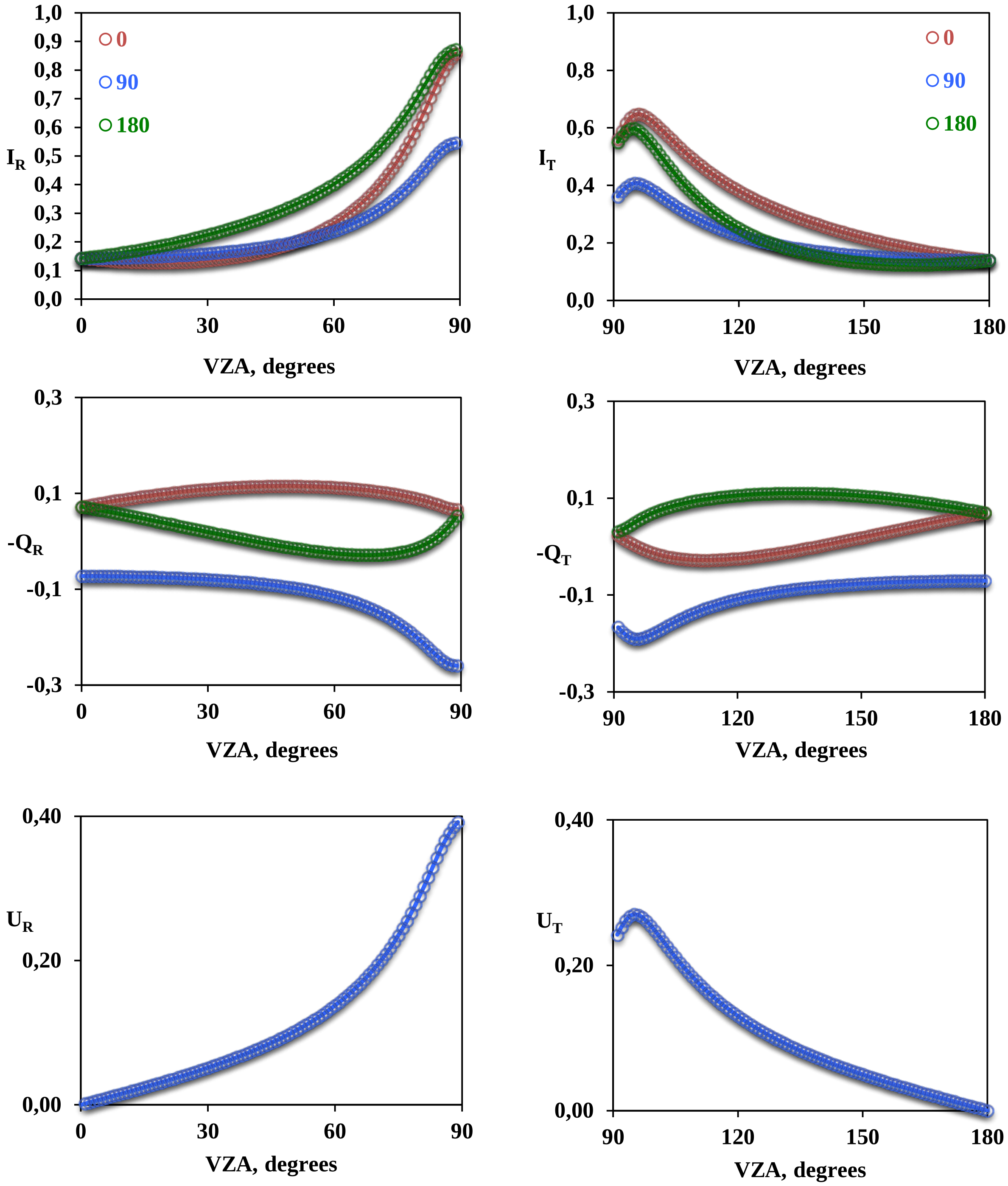

Fig. 5: The normalized Stokes vector for the Rayleigh layer in the reflected and transmitted radiation (line – SCIATRAN, circles – polarized MC). The solar zenith angle is 60^o the RRA are 0^o, 90^o and 180^o and measured counter clock-wise.

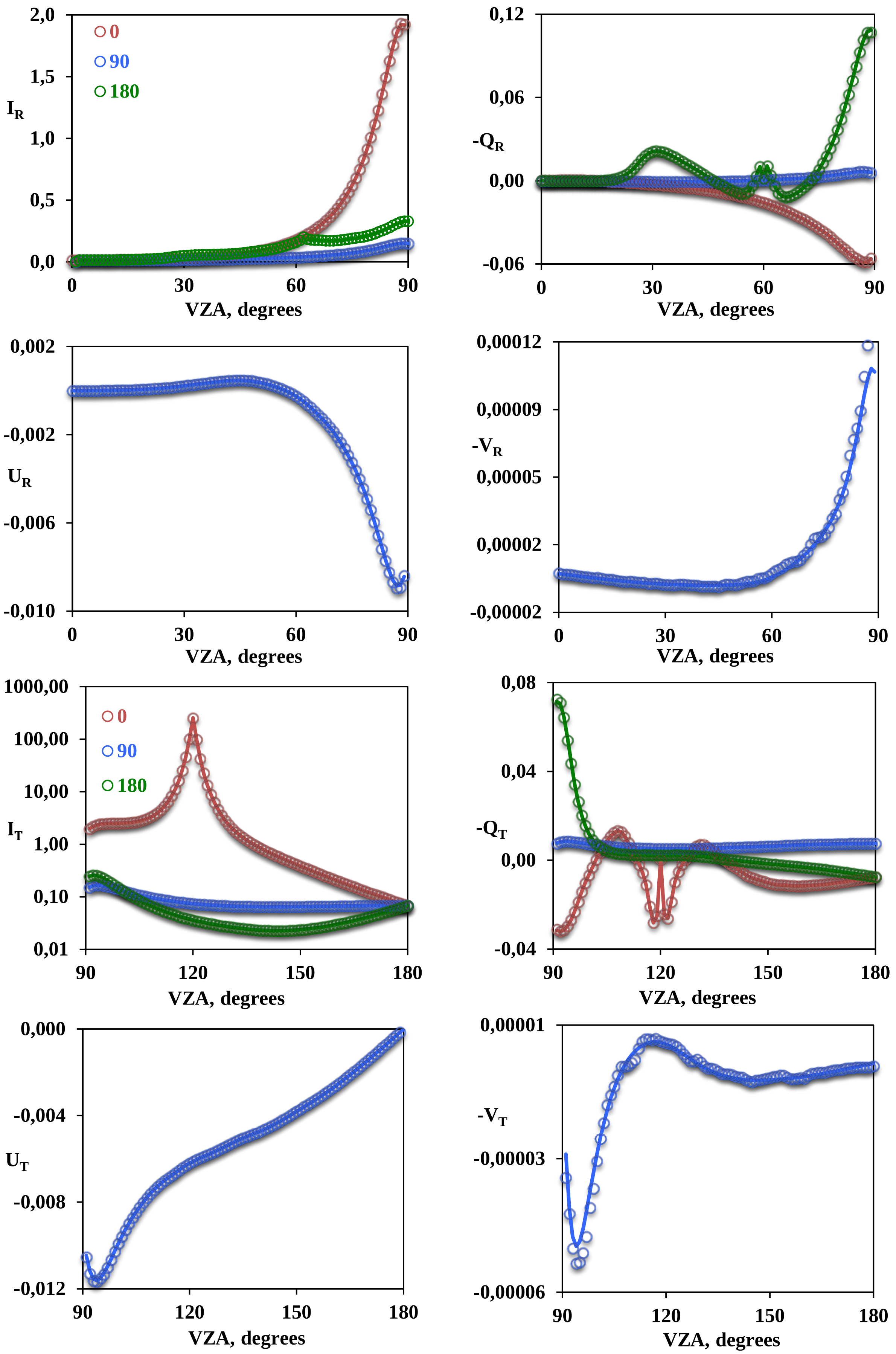

Fig. 6: The same as in Fig. 5 but for the aerosol layer.

The relative differences of our results for the first three components of the Stokes vector as correlated to the benchmark results were also calculated. Where the values of the Stokes components tend to zero are ignored as they can lead to large values of the relative difference. There is an excellent agreement between the polarized MC model and the output from SCIATRAN for the molecular scattering. Note here that the fourth Stokes parameter is always zero for this case, and it disappears at relative azimuth angles of 0^o and 180^o. Relative differences are less than 0.2% for the first Stokes element, and up to 2.5% for the Q and U (for the used number of photons, 10^7). Furthermore, the comparison for the aerosol layer pointed out that the polarized MC model produces accurate results for the first three components of the Stokes vector for both reflected and transmitted radiation. The relative differences are less than 1.2% for the first Stokes component I, and up to 1% and 5% for the Q and U respectively (for the used number of photons, 10^8). However, for the last component *V* we could clearly identify a notable noise. This is due to the fact that calculation is statistical in the Monte Carlo method; results are always subject to statistical uncertainty. In addition, in order to ameliorate such problem and correctly derive the component *V*, more than 10^{10} photons should be selected for the simulations, which dramatically increases the simulation time.

For rather irregular particles, we compared our polarized MC model against the tabulated values by Wauben and Hovenier (1992), retrieved by two different computational ways (i) a doubling/adding method (de Haan et al., 1986) and (ii) the F_N method (Garcia et al., 1989). In this study, we will present only the results obtained for the atmospheric model 1 (Kuik et al., 1992), which corresponds to a homogeneous plane-parallel atmosphere with a layer of randomly oriented prolate spheroids with a refractive index 1.55 – 0.01i above an ideal absorbing surface. The comparison is illustrated in Fig. 7. Simulations were conducted for an incident unpolarized flux of π at a solar zenith angle of 53.13 degrees and two different RRA (0^o and 90^o). The cloud optical thickness and the single scattering albedo are both one.

In the polarized Monte Carlo model the number of photons selected was 10^7. It should be noted that the third and fourth element of the Stokes vector disappears for a RRA=0^o for both reflected and transmitted radiation. There is a very good agreement with the benchmark results for the parameters *I, Q, U* (relative differences are less than 6%). On the other hand, the efficiency of the polarized model is not enough to calculate the last component *V* for highly irregular particles, since it could get very small values.

To this end, the comparisons proved that our model can handle multiple scattering with high efficiency and is able to calculate polarized radiances for all the different particle cases.

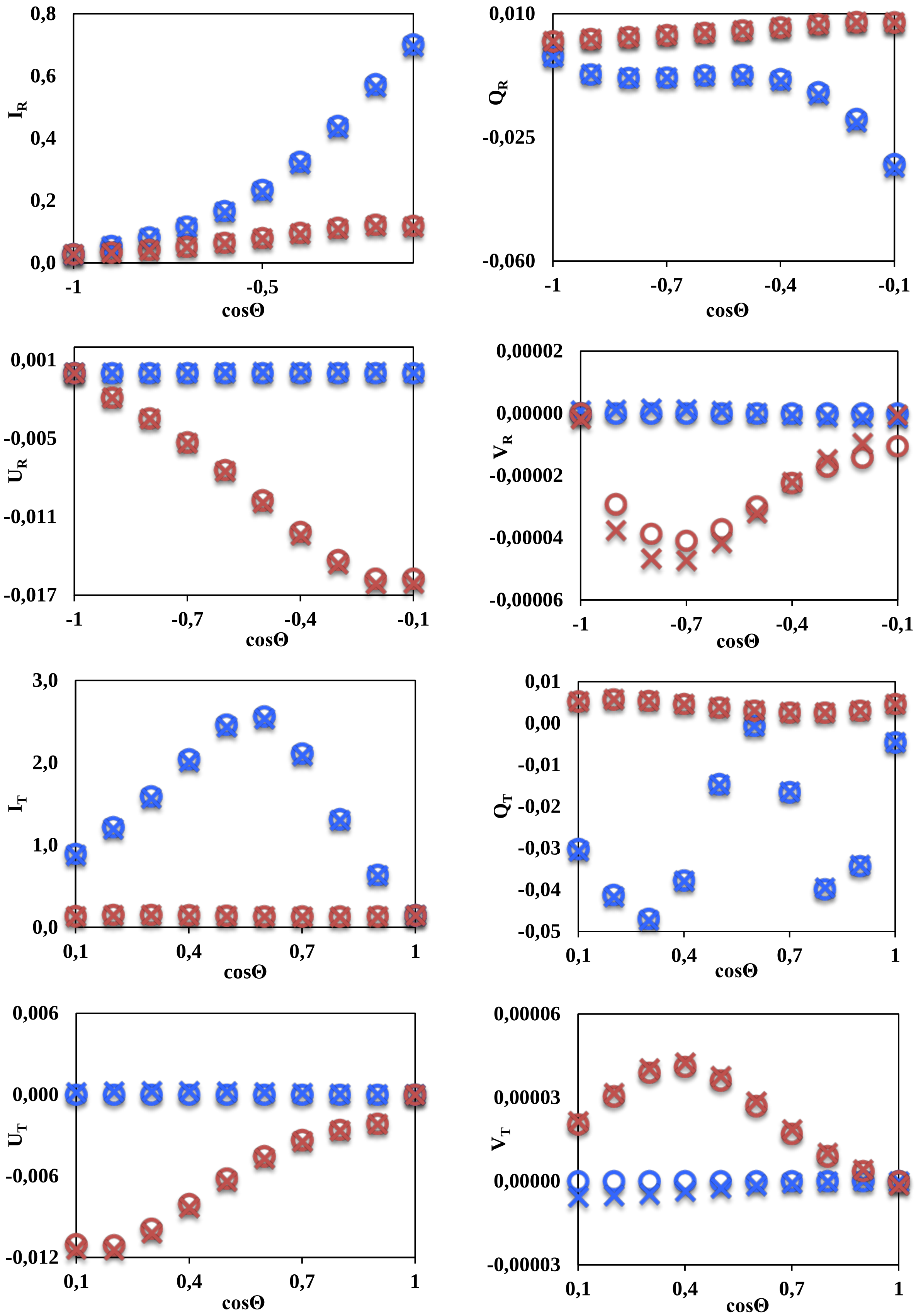

Fig. 7: The normalized Stokes vector for a layer of randomly oriented prolate spheroids in the reflected and transmitted radiation (circles – Wauben and Hovenier, crosses – polarized MC). The cosine of the solar zenith angle is 0.60 and the relative azimuth angles are 0° (blue markers) and 90° (red markers).

4. Summary and outlook

The present study has described the implementation of polarization into a 3D Monte Carlo radiative transfer model. It employs the statistical Monte Carlo technique (in the forward scheme) and it is designed to calculate column-response pixel-based polarized radiative densities for 3D inhomogeneous cloudy atmospheres. The biased-sampling method introduced in this study is perhaps the fastest approach of the different methods to the polarized radiative transfer problem. Furthermore, in order to allow accurate calculations and diminish the noise of radiance estimations for highly asymmetric phase matrices the Local Estimate Method has been applied.

Validations of the model output for three different cases (Rayleigh scattering, aerosol and randomly oriented prolate spheroids) have been carried out against benchmark results (Kokhanovsky et al., 2010 and Wauben et al., 1992), indicating an excellent agreement. All deviations found for the last component of the Stokes vector for the aerosol case and the layer of randomly oriented prolate spheroids can be explicated by the noise of the MC method in radiance calculations. Increasing the selected number of photons could reduce the noise.

Further comparisons will be conducted against benchmark results for a homogeneous layer above a Lambertian surface (Coulson et al., 1960). Moreover, it is planned to perform sun-photometer-based observations of downwelling solar radiances polarized by Saharan dust and ice particles. The measured data sets will be used and interpreted by means of our polarized radiative transfer model.

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