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Comparison of Monte Carlo simulations with exact Maxwell solutions for polarized light scattering by multiple absorbing spheres

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Abstract. The goal of this study was to investigate the differences between radiative transfer theory and Maxwell theory for simulation of light propagation in a turbid medium. Polarization effects as well as absorbing scatterers with complex index of refraction are taken into account. The simulation volume contained different numbers of scattering and absorbing spheres (radius: 1 μm) and was irradiated from one side with a plane electromagnetic wave ($\lambda = 600 \text{ nm}$). The absorption was varied as well as the concentration of the scatterers. The resulting 16 Müller matrix elements were compared for the Monte Carlo method as well as for the Maxwell method for all scattering angles. An increasing absorption of the spheres resulted in larger differences especially for the intensity results (M_{11} Müller matrix element) between the two solution methods, while increasing scatterer concentrations led generally to larger differences for all Müller matrix elements. That means that the results of radiative transfer theory have to be treated with care for high scatterer concentrations and large absorption. By using the presented method, differences between the two theories can be investigated for arbitrary particle size parameters (spheres) and optical properties of the scatterers.

1. Introduction

The investigation of polarized light propagation in turbid media is an important topic in different research areas as for example in biomedical optics [1, 2]. Maxwell theory can be used for an exact calculation of polarized light propagation in scattering media. However, the problem of this method are extremely high computational needs to investigate relevant simulation volumes, which makes it inappropriate for many applications.

Radiative transfer theory is an approximation of Maxwell theory, allowing to study light propagation also in more extended simulation volumes of scattering media. Polarization dependence as well as absorbing scatterers with complex refractive index can be considered by this approach. However, due to the approximative manner of radiative transfer theory neglecting the wave character of light, there are possible sources of errors which have not been fully investigated until now [3].

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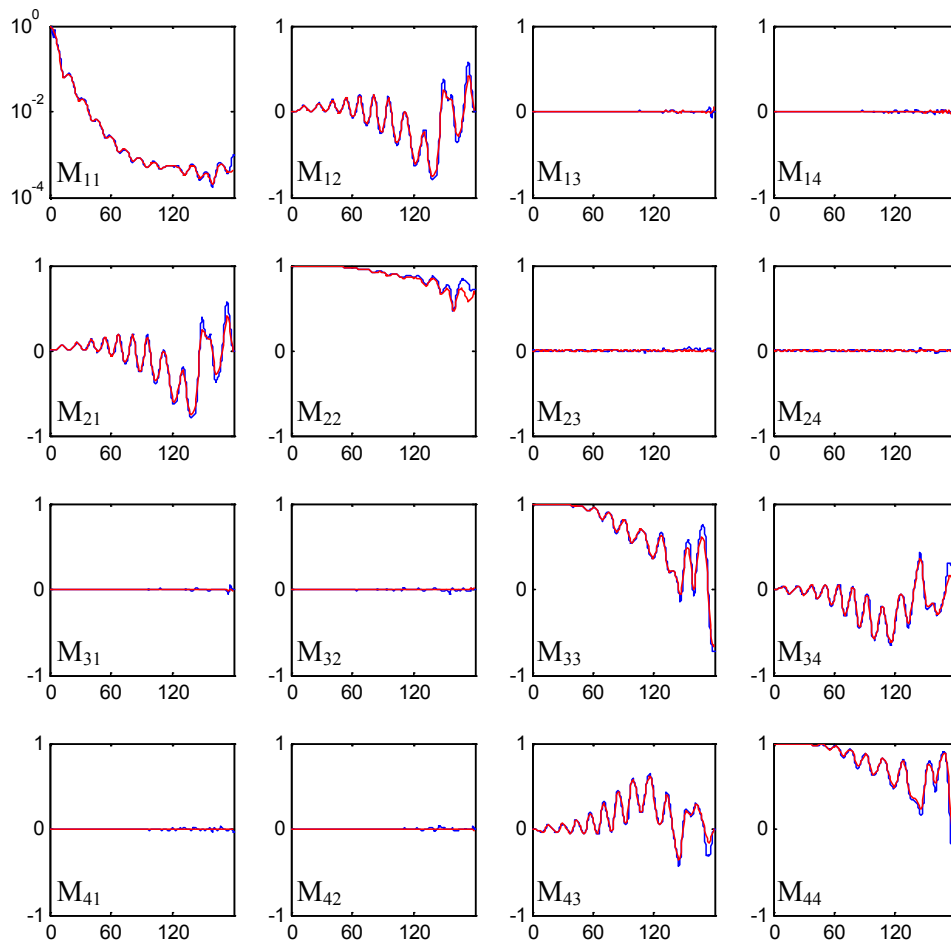


Figure 1. Angularly resolved Müller matrix elements for scattering angles θ ($0^\circ \leq \theta \leq 180^\circ$), $f_v = 5.03$ Vol.-% (12 spheres), $n_{\text{sphere}} = 1.59 + 0.01i$, Monte Carlo method (red) and Maxwell method (blue).

The goal of this study was to investigate the differences between radiative transfer theory and Maxwell theory considering polarization as well as absorbing scatterers. The complete Müller matrix was calculated for several configurations.

2. Material and Methods

A cubic simulation volume ($10 \mu\text{m} \times 10 \mu\text{m} \times 10 \mu\text{m}$) containing different numbers ($N = 12, 24, 48$ and 96) of scattering spheres (radius: $r = 1 \mu\text{m}$) was modelled corresponding to different scatterer concentrations ($f_v = 5.03$ Vol.-%, 10.05 Vol.-%, 20.11 Vol.-% and 40.21 Vol.-%). The refractive index of the infinite outer medium was $n_m = 1.33$ while the refractive index of the scatterers was varied ($n_{\text{sphere}} = 1.59+0.00i$; $1.59+0.01i$ and $1.59+1.00i$). The simulation volume was irradiated by a plane electromagnetic wave with vacuum wavelength $\lambda = 600$ nm.

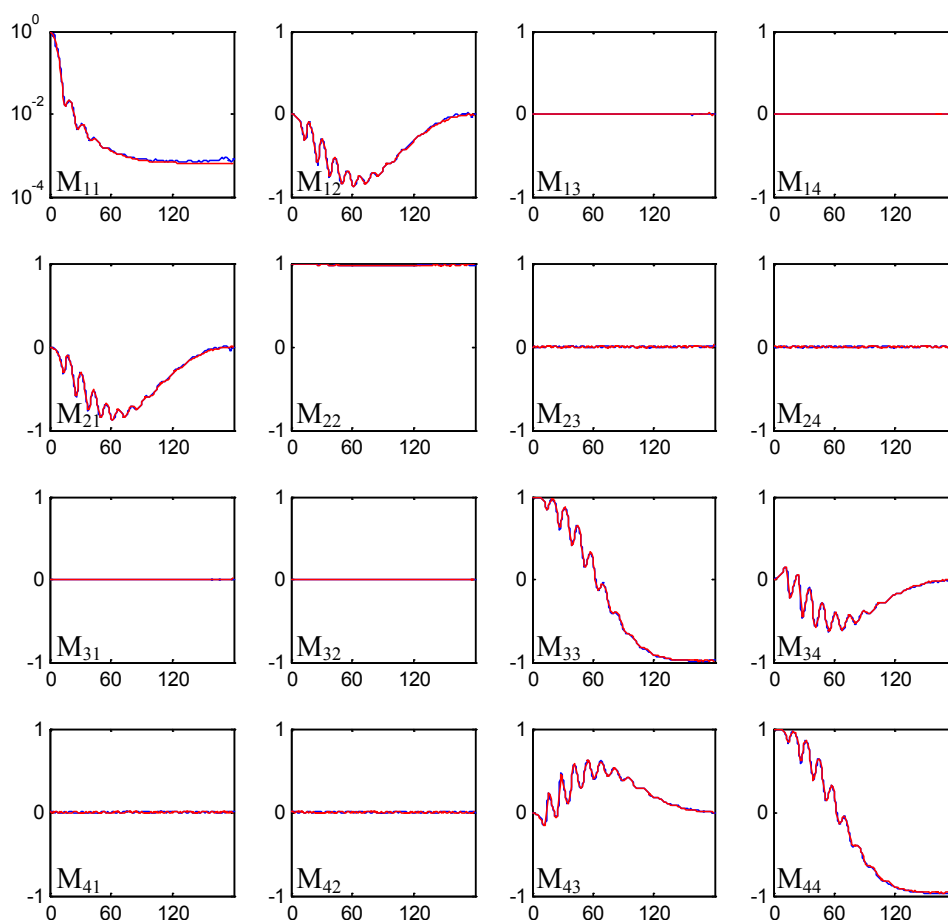


Figure 2. Angularly resolved Müller matrix elements for scattering angles θ ($0^\circ \leq \theta \leq 180^\circ$), $f_v = 5.03$ Vol.-% (12 spheres), $n_{\text{sphere}} = 1.59 + 1.00i$, Monte Carlo method (red) and Maxwell method (blue).

The angular dependent scattering properties (all 16 Müller matrix elements) of the cuboidal simulation volume were calculated by two methods based on the radiative transfer theory and the Maxwell theory, respectively.

The first method consists of a combination of the radiative transfer theory and Mie theory and was solved by a Monte Carlo (MC) program, which was developed by us for this purpose [3-12]. The single sphere Mie solution [13] was used as phase function for the Monte Carlo program. The scattering coefficient μ_s and absorption coefficient μ_a are needed as input for the Monte Carlo program. They were calculated by the Mie formalism as well and depend on the volume fraction of the spheres and their complex refractive index.

An assumed volume fraction of the spheres dispersed in the medium of 5.03 % (12 spheres) with $n_{\text{sphere}} = 1.59 + 0.01i$ ($n_{\text{sphere}} = 1.59 + 1.00i$) led to $\mu_s = 96.18 \text{ mm}^{-1}$ and $\mu_a = 12.39 \text{ mm}^{-1}$ ($\mu_s = 47.63 \text{ mm}^{-1}$ and $\mu_a = 38.62 \text{ mm}^{-1}$). Table 1 shows the calculated absorption and scattering coefficients for all cases.

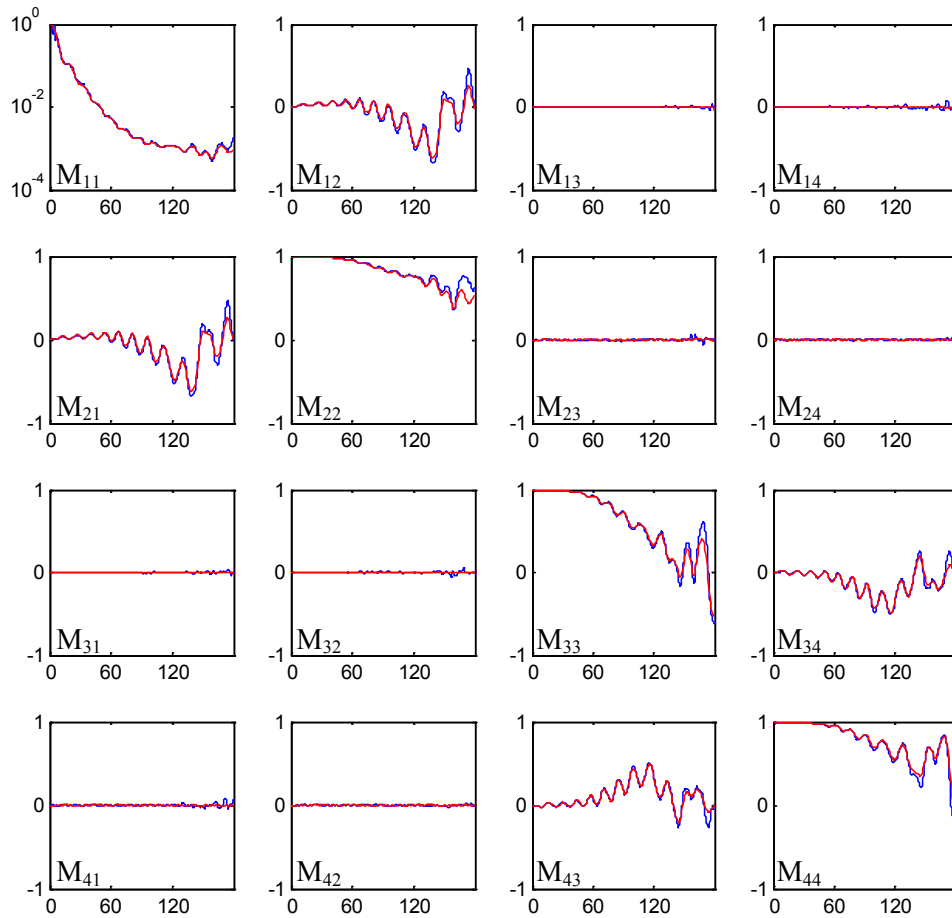


Figure 3. Angularly resolved Müller matrix elements for scattering angles θ ($0^\circ \leq \theta \leq 180^\circ$), $f_v = 10.05$ Vol.-% (24 spheres), $n_{\text{Sphere}} = 1.59 + 0.01i$, Monte Carlo method (red) and Maxwell method (blue).

Table 1. Absorption and scattering coefficients used as input for the Monte Carlo program.

Number of spheres	Volume concentration	n_{Sphere}	μ_a [mm^{-1}]	μ_s [mm^{-1}]
12	5.03 %	$1.59 + 0.01i$	12.39	96.18
12	5.03 %	$1.59 + 1.00i$	38.62	47.63
24	10.05 %	$1.59 + 0.01i$	24.77	192.36
24	10.05 %	$1.59 + 1.00i$	77.24	95.26
48	20.11 %	$1.59 + 0.01i$	49.54	384.72
48	20.11 %	$1.59 + 1.00i$	154.47	190.52
96	40.21 %	$1.59 + 0.01i$	99.09	769.43
96	40.21 %	$1.59 + 1.00i$	308.94	381.04

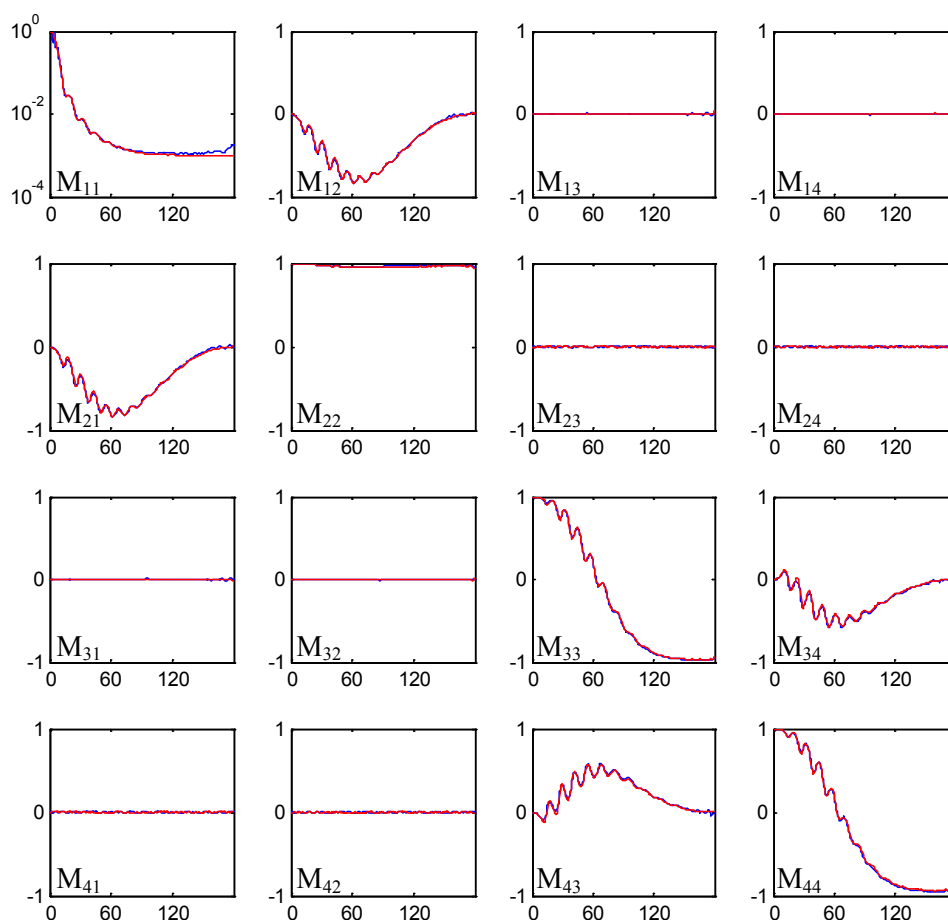


Figure 4. Angularly resolved Müller matrix elements for scattering angles θ ($0^\circ \leq \theta \leq 180^\circ$), $f_v = 10.05$ Vol.-% (24 spheres), $n_{\text{sphere}} = 1.59 + 1.00i$, Monte Carlo method (red) and Maxwell method (blue).

Using these input data, the light scattering problem was solved by the Monte Carlo method and registration of the scattering angle of each photon resulted in the angularly resolved Müller matrix after averaging over the azimuthal ϕ angle.

The second method is provided by a solution of the Maxwell theory (Generalized Multisphere Mie) [14]. Different volume concentrations were modelled by spatial distributions of different numbers of spheres ($N = 12, 24, 48$ or 96 , as in the first method) in a cubic simulation volume where no overlapping of the spheres was allowed. This model was used to calculate the angularly resolved Müller matrix using the same parameters as above (simulation volume: $10 \mu\text{m} \times 10 \mu\text{m} \times 10 \mu\text{m}$, $r = 1 \mu\text{m}$, $n_m = 1.33$, $n_{\text{sphere}} = 1.59+0.00i, 1.59+0.01i$ and $1.59+1.00i$, $\lambda = 600 \text{ nm}$). The results were averaged over 10 randomly generated spatial distributions of the spheres in the simulation volume leading to a reduction of interference speckles.

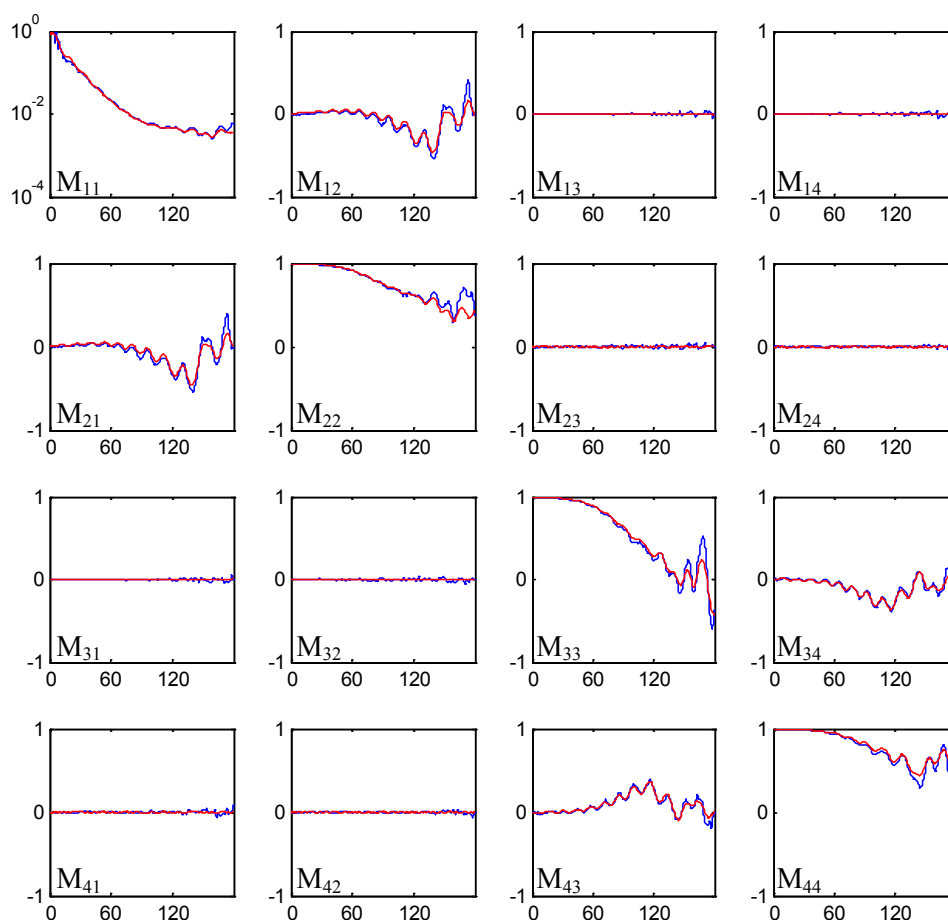


Figure 5. Angularly resolved Müller matrix elements for scattering angles θ ($0^\circ \leq \theta \leq 180^\circ$), $f_v = 20.11$ Vol.-% (48 spheres), $n_{\text{sphere}} = 1.59 + 0.01i$, Monte Carlo method (red) and Maxwell method (blue).

For both methods, the normalized form of the Müller matrix was used for representation of the calculated scattering characteristics. Therefore, all elements except M_{11} itself were normalized to M_{11} for each scattering angle. The M_{11} element was normalized to forward direction values of the Monte Carlo solution in both cases. This enabled a direct comparison of the angular variations as well as the absolute values of the scattering characteristics between the two approaches.

3. Results and discussion

Radiative transfer theory (Monte Carlo solution) as well as Maxwell theory have been applied to calculate all Müller matrix elements for comparison.

Figures 1-8 show the angular dependent 16 Müller matrix elements versus the scattering angle θ in the range from 0 to 180 degrees for different scatterer concentrations and for different imaginary parts of the scatterer refractive index. The results of the Monte Carlo simulations as well as of the Maxwell solutions are shown in each figure.

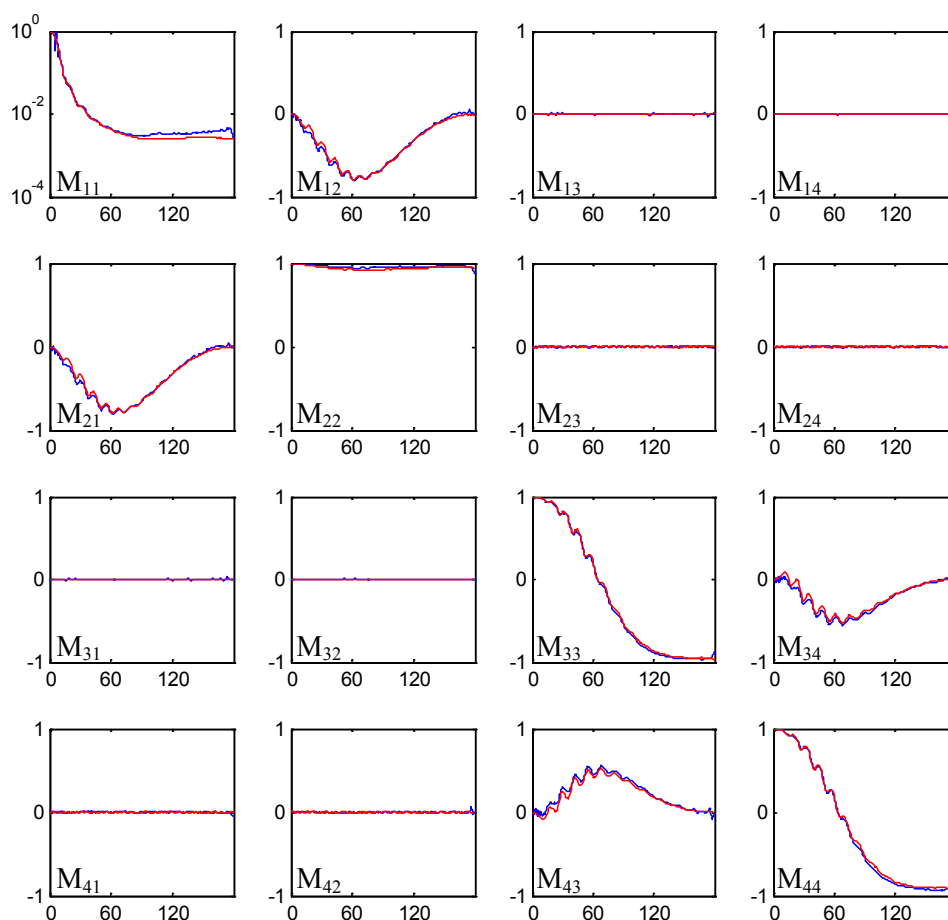


Figure 6. Angularly resolved Müller matrix elements for scattering angles θ ($0^\circ \leq \theta \leq 180^\circ$), $f_v = 20.11$ Vol.-% (48 spheres), $n_{\text{Sphere}} = 1.59 + 1.00i$, Monte Carlo method (red) and Maxwell method (blue).

The results for $n_{\text{Sphere}} = 1.59 + 0.00i$, which are not given here, show a similar behaviour as the results for $n_{\text{Sphere}} = 1.59 + 0.01i$ (figures 1, 3, 5 and 7) for all concentrations and all Müller matrix elements, whereas the quantitative values of the intensity (M_{11} element) for $n_{\text{Sphere}} = 1.59 + 0.00i$ exceed the values for $n_{\text{Sphere}} = 1.59 + 0.01i$.

The overall shape of the Müller matrix remains roughly similar for all concentrations for $n_{\text{Sphere}} = 1.59 + 0.01i$ (figures 1, 3, 5 and 7) as well as for $n_{\text{Sphere}} = 1.59 + 1.00i$ (figures 2, 4, 6 and 8). However, large differences in Müller matrix structure can be observed between the two different refractive indices. In case of a small imaginary part of the refractive index, a strong dependence on the scattering angle can be observed while in the backscattering region the Müller matrix approximates the properties of a half-wave plate in case of a high imaginary part of the refractive index. This means, that the matrix approaches a diagonal matrix with $M_{22} = 1$, $M_{33} = -1$ and $M_{44} = -1$ for these angles.

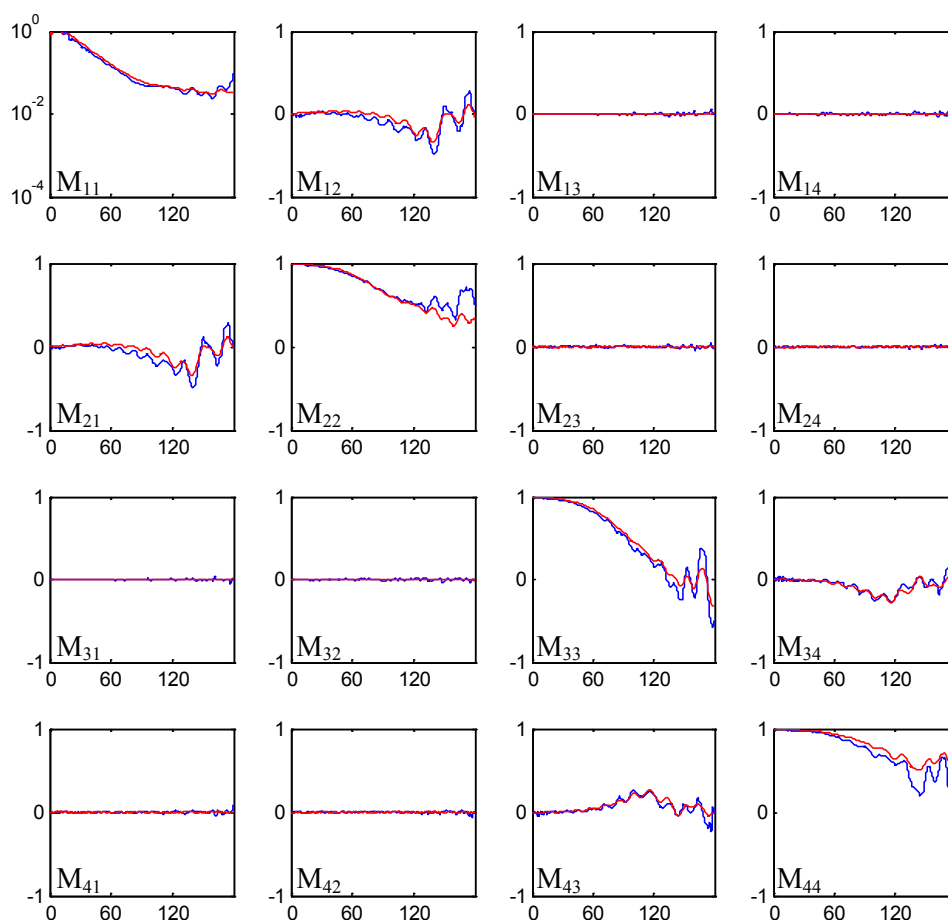


Figure 7. Angularly resolved Müller matrix elements for scattering angles θ ($0^\circ \leq \theta \leq 180^\circ$), $f_v = 40.21$ Vol.-% (96 spheres), $n_{\text{sphere}} = 1.59 + 0.01i$, Monte Carlo method (red) and Maxwell method (blue).

In case of small concentrations more oscillations over the scattering angle θ can be observed for both refractive indices. These oscillations result from the single Mie solution and decrease with increasing scatterer concentrations. This effect is visible for both solution methods and is mainly attributed to multiple scattering.

The differences between radiative transfer theory and Maxwell theory which are visible especially for the M_{11} element in the low angle range ($\theta \leq 10^\circ$) are due to forward interferences and result from the limited simulation volume. This effect was already described for unpolarized [15] and polarized light [3] for non-absorbing scatterers and was now observed for absorbing scatterers (non-zero imaginary part of the index of refraction) here. The peak near 180 degrees (visible in the M_{11} element) results from coherent backscattering [16]. Dependent scattering effects cannot be described by the classical radiative transfer theory and are thus a further source of differences to the exact Maxwell theory as was already described in literature [17, 18]. These differences are mostly visible for high scatterer concentrations.

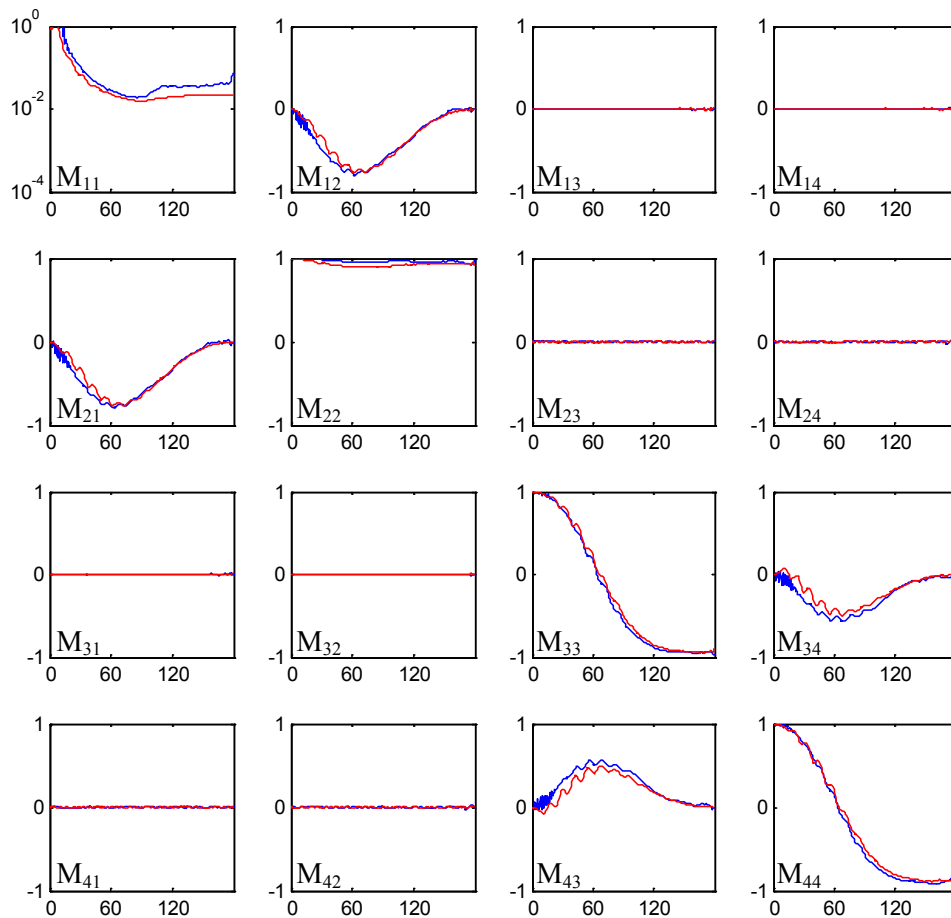


Figure 8. Angularly resolved Müller matrix elements for scattering angles θ ($0^\circ \leq \theta \leq 180^\circ$), $f_v = 40.21$ Vol.-% (96 spheres), $n_{\text{sphere}} = 1.59 + 1.00i$, Monte Carlo method (red) and Maxwell method (blue).

An interesting behaviour of the M_{11} element can be seen for angles $\theta > \approx 90^\circ$ in case of $n_{\text{sphere}} = 1.59 + 1.00i$ which becomes more pronounced if high scatterer concentrations are taken into account: the Maxwell solution of the M_{11} element strongly deviates from the Monte Carlo solution in this angular range. This effect is not visible for a small imaginary part of the refractive index of the spheres.

A good agreement was observed between the two theories for all Müller matrix elements, especially for small concentrations. An increasing absorption of the scattering spheres showed larger differences in intensity results between the two methods. Also, increasing scatterer concentrations within the medium cause larger errors, due to dependent scattering. That means, that the results of radiative transfer theory have to be treated with care for higher scatterer concentrations. It was also found, that the differences between the two theories depend not only on the concentration and index of refraction, but also on the polarization (individual Müller matrix elements).

4. Conclusions

When polarized light propagation has to be simulated using radiative transfer theory, one has to pay attention to possible sources of errors if high scatterer concentrations or strongly absorbing particles are to be considered. A variation of the scatterers imaginary part of the refractive index between 0.01i and 1.00i showed a very different behaviour of the Müller matrix elements.

By the presented method, differences between the two theories can be investigated for arbitrary particle size parameters (spheres) and optical properties of the scatterers.

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