Anisotropic Light Diffusion: An Oxymoron?

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Light propagation in anisotropic random media is studied in the steady-state and time domains. Solutions of the anisotropic diffusion equation are compared to results obtained by the Monte Carlo method. Contrary to what has been reported so far, we find that even in the "diffusive regime" the anisotropic diffusion equation does not describe correctly the light propagation in anisotropic random media.

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Anisotropic light propagation has been studied in a variety of random media, for example, in nematic liquid crystals [1,2], in biological tissue [3], or in etched gallium phosphide [4,5]. In many biological tissues the light propagation is anisotropic, for example, in muscle, skin, tendon, ligament, neural tissue, bone, enamel and dentin [3,6–8].

For the theoretical description of the anisotropic light propagation in random media usually solutions of the anisotropic diffusion equation were used. In general, the diffusion equation can be derived from the more exact radiative transport equation assuming that the angular distribution of the radiance is only slightly anisotropic [9]. This condition is fulfilled in the so called diffusive regime, that means at positions far from the light source and boundaries, and at times sufficiently long after the incidence of the light beam.

The anisotropic diffusion equation was derived from the transport theory by several groups [10–13]. Although good agreement between the anisotropic diffusion equation and experiments was reported [1,2,4], the validity of the anisotropic diffusion equation is questionable, because in its derivation it is assumed that the angular light distribution is almost isotropic. Thus, the question arises, if anisotropic diffusion is an oxymoron, a contradiction in terms.

In order to investigate this issue we compared the solutions of the anisotropic diffusion equation in the steady state and time domains with results obtained by the Monte Carlo method, which is a numerical solution of the radiative transport equation. We show that large differences exist in both domains. In addition, we point out why an apparent agreement was found in the literature so far.

The anisotropic diffusion equation is given by

$$\frac{1}{c}\frac{\partial\Phi(\vec{r},t)}{\partial t} - \mathbf{D}\nabla^2\Phi(\vec{r},t) + \mu_a\Phi(\vec{r},t) = S(\vec{r},t), \qquad (1)$$

where $c = c_0/n_m$ is the light velocity in the random medium having a refractive index n_m and c_0 is the light velocity in vacuum. Φ is the fluence rate, μ_a the absorption coefficient, S the source, and $\mathbf{D}$ is the diffusion tensor [13,14]. In the following it is assumed that only the diagonal components of $\mathbf{D}$, D_x, D_y, D_z, are not zero, that means that the alignment of the microstructure of the random medium is along one of the coordinate axes. We consider a slab with a thickness d and laterally infinite extensions. The pencil light beam is incident perpendicular to the slab boundary in z-direction at $x = y = 0$ mm. The reduced scattering coefficients in directions of the coordinate axes are $\mu'_{si} = 1/(3D_i)$.

It can be shown using a simple rescaling that the solutions of the isotropic diffusion equation can be used to obtain the solutions of the anisotropic diffusion equation in the time and steady-state domains [4]. We calculated the time-resolved transmittance, $T(t)$, and the spatially resolved transmittance, $T(x, y)$, from the slab by using Fick's law at the lower boundary: $T = D_z \frac{\partial\Phi}{\partial z}|_{z=d}$ [15].

In the Monte Carlo method the anisotropic light propagation can be implemented in different ways. We programmed the version that is closest to the assumptions used in the derivation of the anisotropic diffusion equation. A standard Monte Carlo code was modified [15] so that the scattering coefficient depended on the propagation direction of the photon. We calculated the average path length of a photon that propagates in direction $\vec{n}$ (given by the polar angle and the azimuthal angle of the spherical coordinates, θ and ϕ, respectively) according to the diffusion tensor of the anisotropic diffusion equation. Using $D_{\vec{n}} = \vec{n}\mathbf{D}\vec{n}^T$, where $\vec{n} = (\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta))$ is the unit vector, the reduced scattering coefficient in direction $\vec{n}$ is obtained with $\mu'_{s\vec{n}} = 1/(3D_{\vec{n}})$. For the phase function (scattering function) we used a Henyey-Greenstein function with an anisotropy factor of $g = 0.8$ independent of the direction of the incoming photons [15]. For random media with a refractive index, n_m, different to that of the surrounding medium, n_o, Fresnel's formula were used.

Besides the above version (termed MCt) we also implemented a Monte Carlo code (termed MCc) that is closer to the physical reality. It was assumed that the scattering medium contained cylindrical structures that were aligned in one direction (here the x direction). The scattering by these cylinders was calculated by solutions of the Maxwell equations [16]. It is found that the angular distribution of the scattered light depends strongly on the incoming direc-

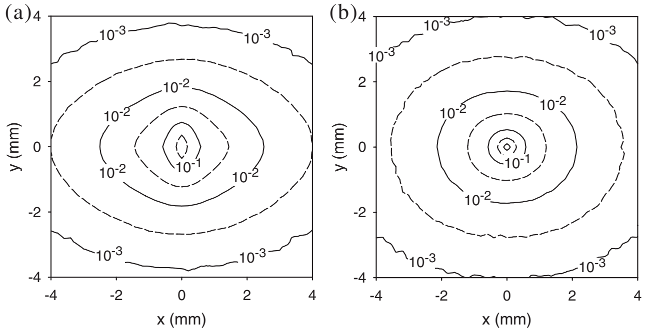

FIG. 1. Spatially resolved reflectance $R(x, y)$ (unit: mm^{-2}) calculated with (a) MCc and with (b) MCt.

tions of the photons relative to the cylinders, which cause an anisotropic light propagation. For the geometrical and optical properties of the cylinders we used those of the dental tubules, which are the main structure of the tooth's dentin [16]. In order to reduce and alter the anisotropy of the light propagation we also added scatterers that scatter light independent on the incident direction using a Henyey-Greenstein function with $g = 0.8$ as phase function, see [16]. The principle approach in MCc is as follows. The photon's path length is calculated using the sum of the scattering coefficients in the propagation direction of the photon for both types of scatterers and the absorption coefficient. Then, using the ratio of these scattering coefficients it is decided, if the photon is scattered by a particle described by the Henyey-Greenstein function or by a cylinder. Finally, the new direction of propagation is computed by applying the appropriate phase function.

Figure 1 compares the spatially resolved reflectance $R(x, y)$ from a semi-infinite turbid medium calculated with MCc, Fig. 1(a), and with MCt, Fig. 1(b). The optical properties used for these simulations were $\mu'_{sx} = 1\ \mathrm{mm}^{-1}$, $\mu'_{sy} = \mu'_{sz} = 2\ \mathrm{mm}^{-1}$, $\mu_a = 0.01\ \mathrm{mm}^{-1}$, which are typical for biological tissue, and $n_m = n_o = 1.0$. For MCc these reduced scattering coefficients were achieved by using scatterers described by the Henyey-Greenstein function with $\mu'_{sx} = \mu'_{sy} = \mu'_{sz} = 1\ \mathrm{mm}^{-1}$ and by changing the concentration of the dental tubules until the reduced scattering coefficients were $\mu'_{sy} = \mu'_{sz} = 1\ \mathrm{mm}^{-1}$ and $\mu'_{sx} = 0\ \mathrm{mm}^{-1}$. This implies that the scattering coefficient due to the cylinders along the cylinders' direction is zero, which follows from the solution of the Maxwell equations.

Figure 1(a) shows that the isointensity contour lines of $R(x, y)$ obtained from MCc are elongated in y direction for small distances and in x direction for long distances from the incidence source due to the scattering characteristics of the cylindrical scatterers [16]. Contrarily, the contour lines in Fig. 1(b) are all elongated in x direction, which is closer to the results obtained from the anisotropic diffusion equation, where the contour lines are ellipses having the same aspect ratio (not shown). Thus, in the following mainly the results of MCt are compared to the solutions of the anisotropic diffusion equation. For these comparisons we used transmittance instead of reflectance data, because the diffusion approximation is better fulfilled in transmission due to the larger distance from the incident source. In addition, a lot of the work in literature have been performed in this geometry.

Figure 2 shows the spatially resolved transmittance from a slab with a thickness of 5 mm. The figures give $T(x, y)$ along the x and along the y directions calculated with MCt (solid curves) and with the solutions of the anisotropic diffusion theory (dashed curves). The optical properties used for Fig. 2(a) were $\mu'_{sx} = \mu'_{sy} = \mu'_{sz} = 2\ \mathrm{mm}^{-1}$, $\mu_a = 0.01\ \mathrm{mm}^{-1}$, $n_m = n_o = 1.0$. For Fig. 2(b) and 2(c) the same optical properties were applied, but μ'_{sx} was changed to $1.6\ \mathrm{mm}^{-1}$ and $1.0\ \mathrm{mm}^{-1}$, respectively.

In Fig. 2(a) the curves in both directions coincide due to the isotropic reduced scattering coefficient. The average relative difference between the Monte Carlo data and the solution of the diffusion equation are $\approx 1\%$, whereas these differences are much larger for the media having anisotropic optical properties [$\approx 8\%$ in Fig. 2(b) and $\approx 15\%$ in Fig. 2(c)].

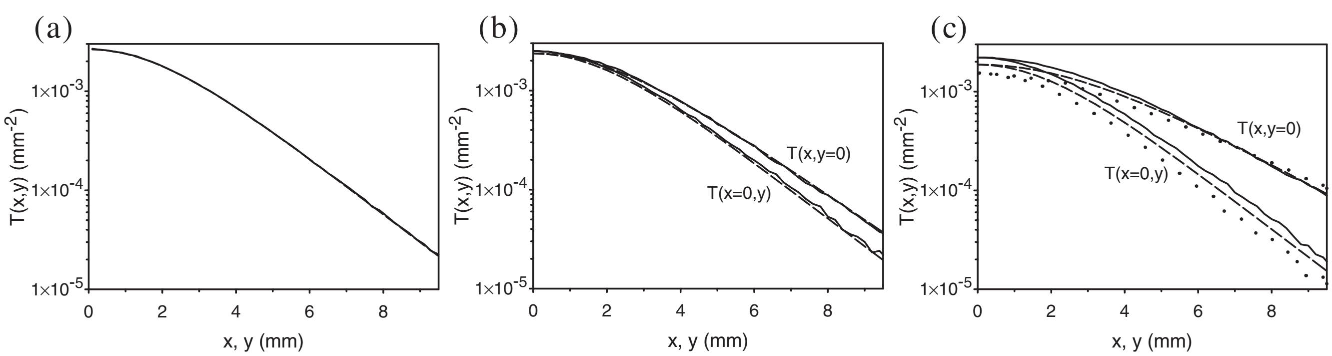

FIG. 2. (a) Spatially resolved transmission along the x and y directions for a slab with $\mu'_{sx} = \mu'_{sy} = \mu'_{sz} = 2\ \mathrm{mm}^{-1}$. In (b) and (c) μ'_{sx} was changed to $1.6\ \mathrm{mm}^{-1}$ and $1.0\ \mathrm{mm}^{-1}$, respectively. Data were calculated with the anisotropic diffusion equation (dashed curves), with MCt (solid curves), and with MCc (dotted curves).

Thus, the errors due to the anisotropic diffusion equation increase by an order of magnitude for typical optical properties found in biological media compared with the isotropic case. This has a decisive impact for the solution of the inverse problem. For media with isotropic optical properties μ_a and μ_s' are obtained from Monte Carlo simulations of $T(x, y)$ within errors of $\approx 10\%$, while for the anisotropic optical properties the errors are unacceptable large (typically $\approx 50\%$ or more). In addition, Fig. 2(c) shows the results for the corresponding MC*c* simulation (dotted curves). It can be seen that the obtained $T(x, y)$ curves do not coincident with MC*t* indicating that the real microstructure has to be considered for an exact description of the light propagation in anisotropic random media. Interestingly, the results of the anisotropic diffusion theory are between those calculated with MC*c* and MC*t*.

Figure 3 shows the time-resolved transmission from a slab with a thickness of $d = 10$ mm at the opposite site of the incident light beam ($x = y = 0$ mm). Two random media with isotropic ($\mu_s' = 1$ mm^{-1} and $\mu_s' = 2$ mm^{-1}) and one with anisotropic reduced scattering coefficients ($\mu_{sx}' = \mu_{sy}' = 1$ mm^{-1}, $\mu_{sz}' = 2$ mm^{-1}) are shown. The other optical properties are $\mu_a = 0.01$ mm^{-1}, $n_m = n_o = 1.0$. $T(t)$ calculated with the MC*t* method (solid lines) and with the solutions of the diffusion theory (dashed lines) are shown.

The time-resolved transmittance from the isotropic random media calculated with diffusion theory agree well with MC*t*. However, large differences are found for the anisotropic random medium. The shape of the time-resolved transmittance calculated with the solution of the anisotropic diffusion equation depends on μ_{sz}', but not on μ_{sx}' or μ_{sy}' [2,4]. Thus, in Fig. 3 the curve for $\mu_s' = 2$ mm^{-1} and that for the anisotropic medium are only different due to a different multiplicative constant in the solution of the anisotropic diffusion equation. However,

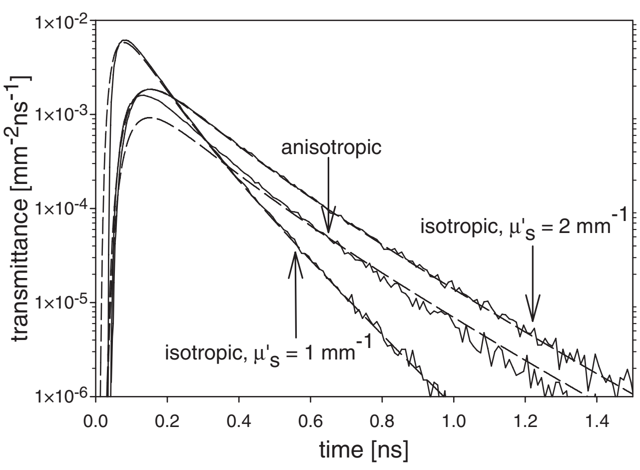

FIG. 3. $T(x = 0$ mm, $y = 0$ mm, $t)$ calculated with MC*t* (solid lines) and solutions of the diffusion theory (dashed line). The detection area in the simulations was $\Delta x \Delta y = 1$ mm^2.

this contradicts intuition, because also μ_{sx}' and μ_{sy}', influence the shape of $T(t)$. This influence can clearly be seen in the Monte Carlo simulations given in Fig. 3. The shape of $T(t)$ from the anisotropic random medium calculated with the Monte Carlo method is, as expected, between those for the two isotropic random media. We note that also for large t-values (for example at $t \approx 1.2$ ns) the solution of the anisotropic diffusion equation does not converge to the Monte Carlo simulations, which is, in general, true for the isotropic diffusion equation in the diffusive regime.

Considering the determination of the optical properties in the time domain, however, we recently found that it is possible even with the solution of the isotropic diffusion equation to obtain accurate values for μ_a from random media having anisotropic optical properties [17].

Finally, we investigated why it has been stated in the literature that, nevertheless, there is a good agreement between experiment and the anisotropic diffusion equation. For example Johnson *et al.* performed a thorough experimental study on a slab of gallium phosphide [4]. This material was etched to obtain a highly scattering random medium having anisotropic optically properties. They measured the spatially resolved transmittance from the random medium and obtained elliptical isointensity contour lines with a ratio of the main axes in x and y directions of about 2. They concluded by using the solution of the anisotropic diffusion equation that μ_{sy}' was 4 times larger than μ_{sx}'. Then, they measured the time-resolved transmittance, and by fitting the solution of the anisotropic diffusion equation the results of the reduced scattering coefficients were confirmed. Thus, they concluded that the anisotropic diffusion equation is a good description of light propagation in anisotropic random media.

In order to reconstruct these results, we performed a Monte Carlo simulation (MC*t*) using the geometrical and optical properties of the investigated material given in [4]: $\mu_{sx}' = 1231$ mm^{-1}, $\mu_{sy}' = \mu_{sz}' = 5100$ mm^{-1}, $\mu_a = 0.00079$ mm^{-1}, $d = 0.31$ mm, $n_m = 1.4$ and $n_o = 1.0$. We found that the ratio of the main axes of the elliptical contour lines of $T(x, y)$ was much lower than 2. Then, we

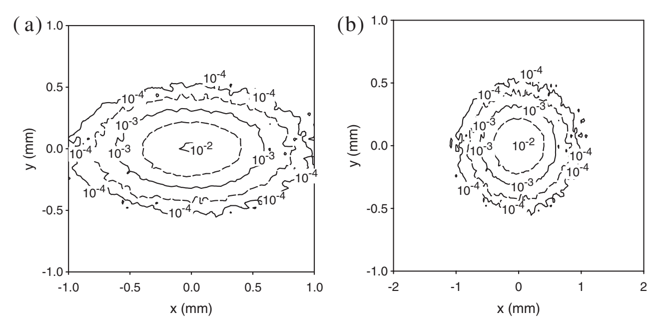

FIG. 4. (a) $T(x, y)$ (unit: mm^{-2}) from a slab with $\mu_{sx}' = 1500$ mm^{-1}, $\mu_{sy}' = \mu_{sz}' = 10\,000$ mm^{-1}, $\mu_a = 0.00079$ mm^{-1}, $d = 0.31$ mm, $n_m = 1.4$ and $n_o = 1.0$; (b) same as (a), but the x axis was multiplied by 2.

changed the reduced scattering coefficients until this ratio was ≈ 2, which was the case for $\mu'_{sx} = 1500\ \text{mm}^{-1}$, $\mu'_{sy} = \mu'_{sz} = 10\,000\ \text{mm}^{-1}$. Figure 4(a) shows the obtained isointensity contour lines of $T(x, y)$. To demonstrate that the ratio of the main axes is ≈ 2, we multiplied the x axis by 2; see Fig. 4(b). It can be seen that the contour lines are close to circles. We note that even more exact circles are obtained for $\mu'_{sy}/\mu'_{sx} \approx 7$, instead of $\mu'_{sy}/\mu'_{sx} = 6.7$.

Following the procedure applied in [4] we, then, fitted the solution of the anisotropic time-resolved diffusion equation to the time-resolved Monte Carlo simulations calculated for the obtained reduced scattering coefficients ($\mu'_{sx} = 1500\ \text{mm}^{-1}$, $\mu'_{sy} = \mu'_{sz} = 10000\ \text{mm}^{-1}$). Similar to [4], we obtained a ratio of the reduced scattering coefficients of ≈ 4. Thus, using the anisotropic diffusion theory we got consistent—but wrong—results in the steady state and in the time domains. Consequently, it is incorrect to conclude from these consistent results that the anisotropic diffusion equation and the determined optical properties are accurate, as the true μ'_{sy}/μ'_{sx} ratio was ≈ 7 and not 4.

In summary, we showed that the diffusion equation for anisotropic random media is much worse than for isotropic random media, restricting strongly its applicability. For the determination of the optical properties of biological tissue in the steady-state domain, for example, prohibitive large errors are obtained, so that solutions of the transport theory, possibly its higher order approximations or random walk models [18] should be used. In general, for an exact description of the light propagation in an anisotropic random medium its microstructure has to be considered, which is not possible with the diffusion approximation. Otherwise, the anisotropic light diffusion might not be an oxymoron for media with a very small anisotropy [compare Fig. 2(b)], because here the condition of an almost isotropic radiance could be fulfilled.

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