

Monte Carlo simulations of coherent backscatter for identification of the optical coefficients of biological tissues *in vivo*

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A Monte Carlo model of light backscattered from turbid media has been used to simulate the effects of weak localization in biological tissues. A validation technique is used that implies that for the scattering and absorption coefficients and for refractive index mismatches found in tissues, the Monte Carlo method is likely to provide more accurate results than the methods previously used. The model also has the ability to simulate the effects of various illumination profiles and other laboratory-imposed conditions. A curve-fitting routine has been developed that might be used to extract the optical coefficients from the angular intensity profiles seen in experiments on turbid biological tissues, data that could be obtained *in vivo*.

Key words: Weak localization, coherent enhancement, Monte Carlo simulations, optical coefficients.

1. Introduction

An accurate knowledge of the optical scattering and absorption properties of biological tissues is fundamental to the understanding of the many uses of light in medicine. This includes both diagnostic techniques such as near-infrared spectroscopy and therapeutic techniques such as photothermal coagulation, photothermal ablation, and photodynamic therapy.^{1,2}

The only technique to be widely accepted for the measurement of the scattering coefficient, μ_s (inverse of the mean-free paths of a photon between scattering events, l_{sc}), and the absorption coefficient, μ_a (inverse of the mean-free path of a photon before absorption, l_a), of a tissue sample is the indirect method of translating diffuse reflectance and transmittance data measured on a slab of tissue by use of either the inverse Monte Carlo³ or the adding-doubling technique.⁴ The major drawback of this method is that it is made postmortem; in addition, the method used to mount the specimen will impose physical effects that almost certainly further influence the optical coefficients. These include the absence of blood, the effects of decay and dehydration following excision,

the shifts in temperature, and the effects of compression.⁵

Several other techniques have been developed that could be used on *in vivo* samples, but none have found widespread use.⁶⁻⁹ A number of these techniques rely on modeling the light transport in tissue with the diffusion approximation, which is valid only for media in which the absorption coefficient is very much less than the scattering coefficient; even then, the results are only valid away from the boundary. This last constraint means that valid results can only be obtained with materials that approximate to large homogeneous volumes and in which the detected signal is not influenced by the measuring apparatus. A fast, noncontact, and highly localized method of tissue characterization that may be used under clinical conditions would be highly desirable.

2. Coherent Backscatter

The basis of radiative transfer theory as attributed to Schuster¹⁰ in 1905 was first extended to include interference effects over multiple mean-free paths by de Wolf¹¹ in 1971. The first observation of a weak localization enhancement cone, caused by the interference effects between two waves propagating through a scattering media along the same routes but with one in reverse order of the other, was seen in a suspension of microlatex spheres in water by Kuga and Ishimaru.¹² The shape of the enhancement cones observed in these experiments was smoothed by the limited angular resolution of the equipment used, but

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this was later improved¹³⁻¹⁵ and gave evidence that supported the theoretical predictions of the line shape made by Tsang and Ishimaru^{16,17} in 1984 and 1985.

A diffusion-approximation derivation that permits a correction to be introduced to compensate for anisotropic scattering and absorption was developed by Akkermans and co-workers in 1986¹⁸ and 1988.¹⁹ Despite the limitations of the diffusion equation to cases in which there are many scattering events and therefore its applicability only to low-absorption cases, and its sensitivity to boundary conditions (particularly refractive index changes and complex geometries), the scalar equation has been frequently used because of its simplicity and supposedly sufficient accuracy.²⁰ A demonstration of the dependence of several established theoretical predictions on anisotropy and boundary conditions was given by Barabanenkov and Ozrin,²¹ with the conclusion that the effects are significant and that the different solutions are not in agreement for highly forward scattering media. The theoretical and experimental evidence of the importance of internal reflections was given by Legendijk *et al.*,²² who showed that higher values of reflectance reduce the full width at half-maximum of the enhancement cone. Gorodnichev *et al.*²³ gave an exact solution for the coherence peak line shape, but only for isotropic scatterers. This overcomes the problems of the single- and double-scattering theory (that of Tsang and Ishimaru¹⁷) and the diffusion-approximation problem of being applicable only to highly scattered events, with the latter problem manifesting itself as inaccuracies in the wings of the cone.

Further experiments went on to show that some backscattered cones were in fact anisotropic, which was attributed by the observers (van Albada *et al.*²⁴) to the low-order Rayleigh multiple scattering that was taking place. A Monte Carlo model was then developed by the same group to validate this theory.^{25,26} Further research was subsequently performed on Monte Carlo simulations within the Mie scattering regime.^{27,28} Much of the subsequent experimental research^{29,30} included time-dependent theories that used picosecond light pulses and various slab geometries to determine the limits of the diffusion equation, and it complemented the research of Etemad *et al.*,³¹ who experimentally compared the similarity in the effects of absorption and limited slab thicknesses. This latter study was the first to attempt extraction of absorption information from samples by a comparison of the line shape of the peak to that obtained with phantoms of identical scattering properties but with zero absorption.

The first attempt to use the coherent backscatter phenomena on biological scatterers was made by Yoo and co-workers,^{32,33} who used picosecond pulses to determine photon path lengths in a way that was similar to their previous research on nonbiological diffusers.^{34,35} Yoo's studies on the biological specimens made comparisons with diffusion-approximation solutions for the coherence peak line shape and came up with absorption and transport scattering

coefficients that were described as similar to results from conventional techniques.

This interest in biological tissue was then taken up by Yoon *et al.*,³⁶ who used a cw laser with a spot size of a few millimeters and a CCD camera detection system along with diffusion-approximation theory to measure transport scattering and absorption coefficients for several *in vitro* tissues. Comparisons were made with data derived by the adding-doubling method of extracting the coefficients from reflectance and transmission measurements with integrating spheres. The results were within likely intersample variations for scattering coefficients but were in error by a factor of 6 for the absorption coefficients. It is our belief that more accurate absorption information would have been achieved if the effects of the finite size of the illuminating beam had been included rather than the inaccurate interpretation of Akkermans' formula.³⁷ The major landmark in this paper was the attempt to use the equipment *in vivo* on a human forearm. It was found that there was no need to rotate the sample to obtain the ensemble or moving averaging that was necessary to get over the speckle pattern from a fixed scattering structure. The *in vivo* averaging is instead obtained by the pulsatile vibrations present in all living tissues. Yoon *et al.*³⁶ suggested that a significant improvement could be obtained by use of a theory other than the scalar theory of Akkermans. The improved theory would encompass the refractive index mismatches and would overcome the diffusion approximation's restriction to high scattering and low-absorption situations. We have developed a Monte Carlo model that takes all of these factors into account.

3. Monte Carlo Model

The equation used to derive the steady-state angular intensity profile, α , for multiply scattered light can be expressed as

$$\alpha = \sum_{\text{all combinations of } i, j} \sum_{\text{all paths } i \rightarrow j} A_i^2 \delta_{ij} + A_j^2 \delta_{ij} + 2A_i A_j \delta_{ij} \cos(\Delta), \quad (1)$$

where the propagator term, δ_{ij} , is the factor by which the photon density falls along the particular path between the possible first and last scattering points, i and j . The terms A_i and A_j represent the amplitude of the light field at the respective points, which is in turn proportional to the square root of the local photon density. The phase term, Δ , is given by the expression

$$\Delta = (\mathbf{R}_i - \mathbf{R}_j) \cdot (\mathbf{k}_0 + \mathbf{k}) = \frac{2\pi n}{\lambda} [x \sin \theta + z(1 - \cos \theta)], \quad (2)$$

where n is the refractive index of the medium, λ is the wavelength of the light *in vacuo*, \mathbf{k}_0 is the incident and \mathbf{k} is the emergent wave vector with angular

separation θ within the medium, and $(\mathbf{R}_i - \mathbf{R}_j)$ is the vector between points i and j with Cartesian components x and z (see Fig. 1). The incident and detected light must be polarized in the same state and preferably with circular polarization.³⁸

In the analytical derivation, incorporation of the propagator term uses the Green's functions within the diffusion approximation. An alternative is to use the established technique of Monte Carlo modeling³⁹⁻⁴² for light being backscattered in the following way. The program traces the individual paths of photons propagating through a scattering medium according to a measured or analytical approximation of a phase function. In this paper the Henyey-Greenstein function was used as an approximation of the scattering phase function⁴³ with various anisotropy factors, g , which are defined as the average cosines of the scattering angles. One sets the distance between random scattering events by taking a random number and using it to sample from a Poisson distribution of the likely scattering lengths. If the photon meets a boundary then the photon is split into two; one is allowed to exit while the other is reflected. The reflected photon has its direction altered and a weight adjusted according to Fresnel laws. If the exiting photon has an emergent direction close to the direction of incidence (within $\sim 10^\circ$), then a record is made in a database of its last scattering position below the free surface in terms of the number of mean scattering free paths from the initial scattering position. Additional parameters such as the photon weight (as decreased by reflection), the total path length, and the number of interactions are also recorded. Photon paths are terminated once the number of scattering interactions exceeds 100,000, where the effects of absorption within tissues can be assumed to have had a dominant effect (see Fig. 2). If the distances are scaled by the mean-free path between scattering interactions and the photon weight is multiplied by the term $\exp(-l\mu_a)$ where l is the path length and μ_a is the absorption coefficient, then the database can be pro-

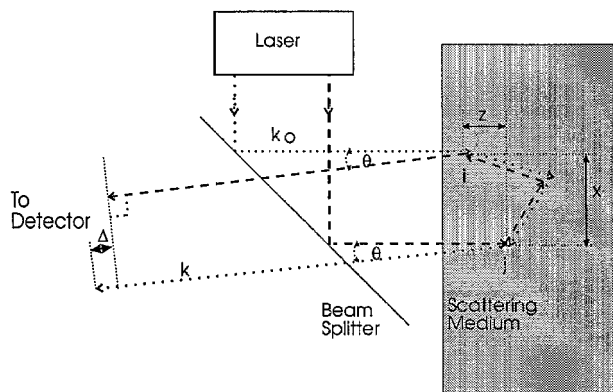


Fig. 1. Coordinate system for backscattered light. Two waves follow an arbitrary path between a first and last pair of scattering points but in opposite directions to one another. The waves emerge along the same direction but out of phase with each other by an amount defined in Eq. (2).

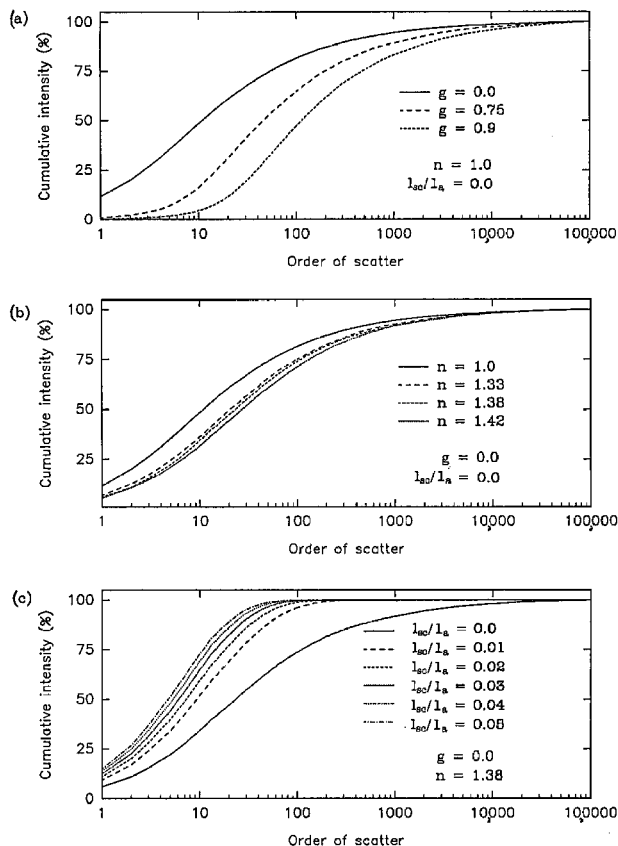


Fig. 2. Cumulative percentage contribution to backscattered light with order of scattering for various transport scattering mean-free path (l_{sc}) to absorption mean-free path (l_a) ratios: (a) effect of anisotropy, (b) effects of a refractive index mismatch between air and tissue, (c) effects of absorption on an isotropic scattering tissue. The cumulative is normalized to that seen after 100,000 interactions.

cessed according to Eq. (1) for any combination of the likely scattering and absorption coefficients that one can expect from tissues.

Several databases were created by use of different combinations of refractive index mismatch and scattering phase function. The databases and their processing were tested when the radial intensity from an incident beam of infinitesimal width was modeled and when the results were compared with those obtained with an analytical time-integrated Green's function solution for light emergent from a point source embedded one scattering mean-free path below the surface.⁴⁴ The two methods showed the same behavior for radial distances in excess of ten mean-free scattering lengths, where the diffusion approximation can be considered to be valid. Several of the databases were analyzed to give graphs of the cumulative intensity as a function of the order of scattering and then normalized to the cumulative intensity after 100,000 interactions. These are shown in Fig. 2. The refractive indices used include that of water (1.33) and a range for tissues (1.38-1.42).⁴⁵ The results shown in Fig. 2(c) indicate that for biological specimens almost all the emergent light is backscat-

tered after experiencing the equivalent of 100 isotropic scattering events, and ~50% emerged after only 5–10 events. This low-order scattering indicates that the diffusion approximation is not suitable for use with coherent backscatter from biological media.

We achieved the modeling of Eq. (1) by considering that all the photon histories in the database had an equal probability of emerging anywhere within the solid angular cone near to the backscatter direction. It is therefore possible to process the database with any set of required scattering and absorption coefficients for any array of angles. The effects of the illumination profile are modeled when this procedure is repeated for a set of initial scattering points covering the illuminating spot. The local intensities can be calculated and translated into amplitude parameters A_i and A_j [Eq. (1)] for the entrance and exit points. Results of this modeling can be seen in Figs. 3, 4, and 5, which also include (where appropriate) the corresponding results of Akkermans' analytical solution derived by use of the diffusion approximation. The abscissa term is defined as

$$q = \frac{2\pi\theta n l_{sc}}{\lambda(1-g)} \quad (3)$$

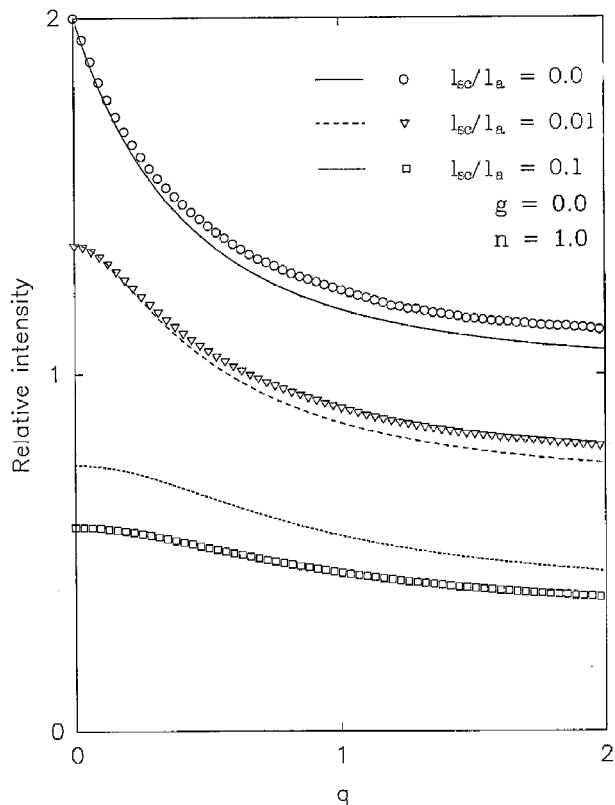


Fig. 3. Effects of absorption on the Monte Carlo predictions together with Akkermans' scalar diffusion-approximation derivation for the coherence peak line shape from multiply scattered light with large diameter beams. The line shapes are relative to the multiply backscattered background level that would have been obtained if the medium were nonabsorbing. The x -axis term is defined in Eq. (3).

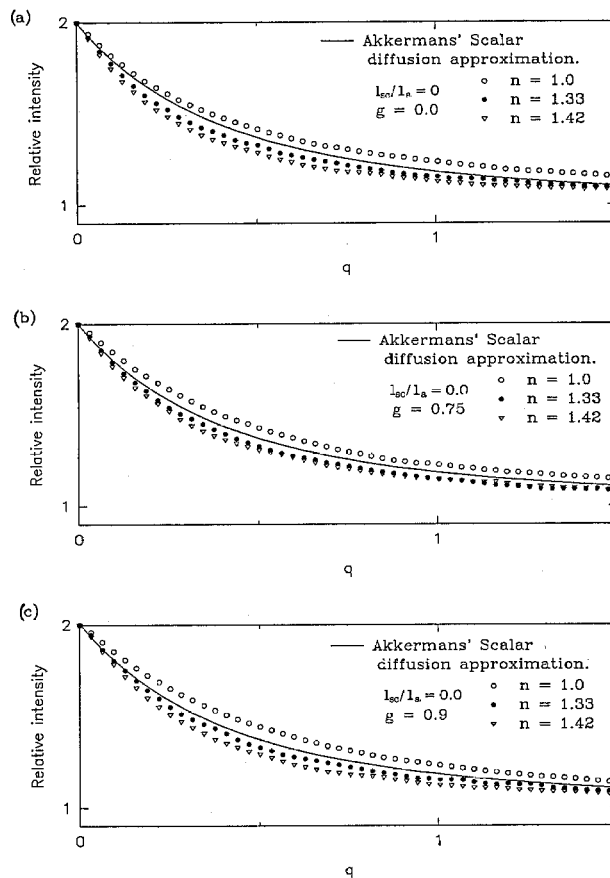


Fig. 4. Effects of a refractive index mismatch and anisotropy on the Monte Carlo predictions together with Akkermans' scalar diffusion-approximation derivation for the coherence peak line shape from multiply scattered light with large diameter beams. The line shapes are relative to the multiply backscattered background level that would have been obtained if the medium were nonabsorbing. The x -axis term is defined in Eq. (3).

The discrepancies seen between the two methods agree with those predicted by Legendijk *et al.*²² and by Barabanenkov and Ozrin²¹ for the effects of refractive index mismatches and nonzero anisotropies. The inability of the diffusion approximation to handle high-absorption cases is clearly evident in Fig. 3 from the large differences between the line shapes from Monte Carlo and Akkermans' methods for the case of $l_{sc}/l_a = 0.1$. The nonuniformity of the illumination profile gives an inequality between parameters A_i and A_j in Eq. (1) and a tendency for the higher orders of scattering not to contribute to the enhancement as much as the incoherent level. This results in the decrease relative to the incoherent contribution and a rounding off of the coherent contribution as seen in Fig. 5. This phenomenon is similar in shape to the effects of illumination with diverging laser beams, and under experimental conditions with biological tissues it is significant.

4. Curve Fitting

To determine the absorption and transport scattering coefficients of the tissue from the Monte Carlo data,

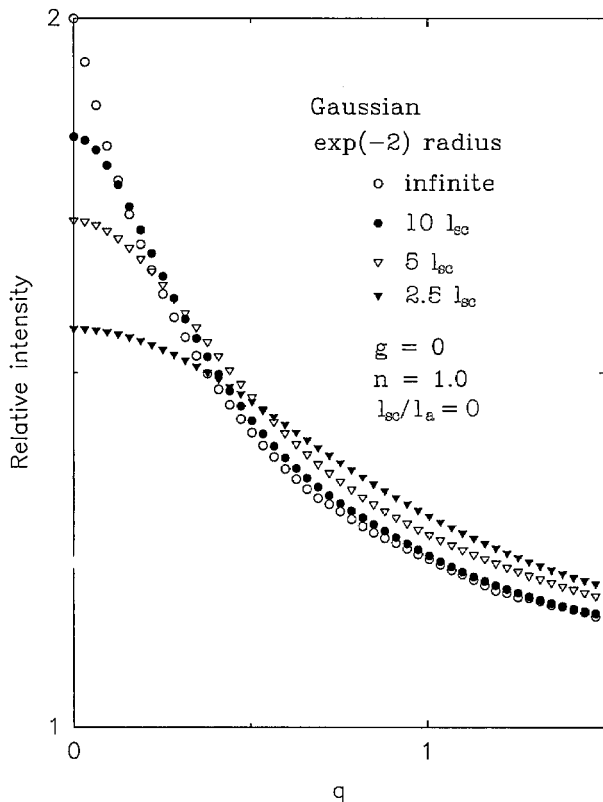


Fig. 5. Results of Monte Carlo simulations of the coherent enhancement of multiply backscattered light from Gaussian profile beams of various radii (radius follows the inverse exponential squared definition). The line shapes are relative to the multiply backscattered background level that would have been obtained if the medium was nonabsorbing. The x -axis term is defined in Eq. (3).

we implemented a Levenberg–Marquardt nonlinear least-squares fitting routine⁴⁶ to fit to the calculated intensity distribution. The routine was used to fit the shape of the curve, its angular offset, and its incoherent intensity relative to what would be obtained without absorption. The fixed parameters fed to the curve-fitting routine are the refractive index mismatch, the beam profile, and the anisotropy factor. These parameters can be measured to a sufficient accuracy with conventional techniques, and in the following simulations they were kept at the same values as used to generate the data. Figure 6 shows the line shape of a coherence peak from a simulation for a highly scattering biological tissue that has had random noise added and then been curve fitted. The noise level in this case was $\pm 7.5\%$ of the background level that would have been obtained with zero absorption. Figure 7 gives an indication of the fitted results and errors obtained from a series of curve-fitting runs on Monte Carlo data calculated with a selection of absorption and scattering coefficients. The process, although computationally intensive (~ 10 min for a Sunsparc 10 workstation), has proved to be sufficiently robust and stable to be used in reconstructing the scattering and absorption coefficients from data with typical experimental noise

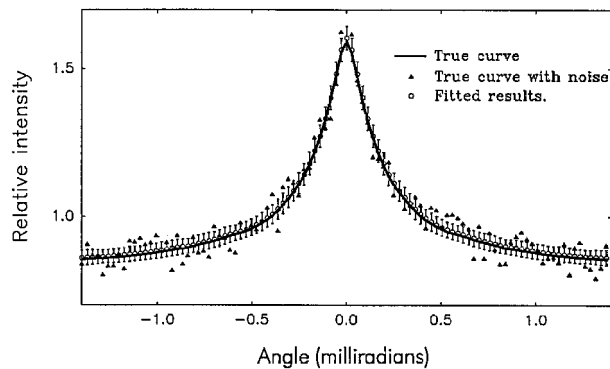


Fig. 6. Graph showing a set of results from the curve-fitting routine. A Monte Carlo simulation is performed for isotropic scattering of 1064-nm light in a medium with a refractive index of 1.0, an absorption coefficient of 0.01/mm, and a scattering coefficient of 2.0/mm. The data are then corrupted with random noise in the range $\pm 7.5\%$ that of the incoherent background level that would have been obtained with zero absorption. A scattering coefficient of 1.99 ± 0.1 /mm and an absorption coefficient of 0.01 ± 0.001 /mm are extracted by use of a nonlinear least-squares fit with μ_a , μ_s , and angular offset as degrees of freedom.

levels, and resolutions similar to those seen in practice (a weighted moving average filter can simulate the effects of a nonperfect system response).³⁶ The results clearly demonstrate the routine's potential to extract scattering and absorption coefficients among random noise.

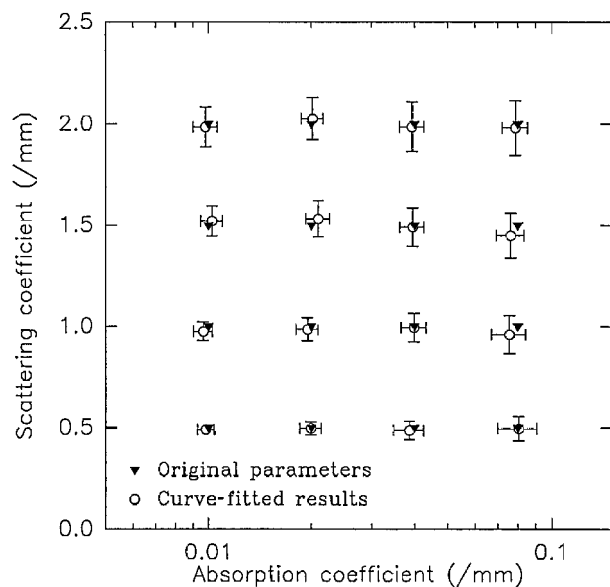


Fig. 7. Results of a series of curve-fitting runs covering a range of absorption and scattering coefficients often found with light at 1064 nm. The original line shape is obtained with a Monte Carlo model for multiply backscattered light with the respective initial coefficients. The angular data consisted of 100 points separated by $28 \mu\text{rad}$. The data are then corrupted with random noise in the range $\pm 5\%$ of the background level that would have been obtained with zero absorption. The curve-fitting routine uses a nonlinear least-squares fit with μ_a , μ_s , and angular offset as degrees of freedom. The error bars indicate the estimated 90% confidence interval obtained with 3 deg of freedom.

5. Conclusion

The range of optical properties found in biological tissues has been shown to be such that it is possible to model backscattered light accurately with Monte Carlo methods that are not too computationally demanding. A model has been developed that produces valid results that can be processed to estimate time-invariant coherence peak line shapes. The discrepancies seen between the Monte Carlo and the diffusion-approximation results agree well with published experimental evidence and the theoretical predictions. The major advantage of this Monte Carlo method is the ease with which it is possible to include additional effects such as various beam profiles and different media geometries. The model has now been included within a curve-fitting program, which has shown a potential ability to determine the optical coefficients of biological tissues with a greater accuracy than has been previously obtained with coherent backscatter. Future research will include experimental validation on phantoms, studies to show the importance of various media geometries and scattering inhomogeneities, and experimental measurements on biological tissues both *in vitro* and *in vivo*.

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