Effect of surface roughness on determination of bulk tissue optical parameters

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Monte Carlo simulations have been conducted to investigate the effect of surface roughness on the inverse determination of bulk optical parameters. Results show that μ_s, μ_a, and g can be overestimated by an order of magnitude for thin slab tissue samples with a moderate index mismatch at the interfaces if typical surface roughness is neglected. Measurements of Intralipid samples between glass windows with smooth and rough surfaces have been carried out and agreement was found between the numerical and the experimental data. This study suggests that the surface roughness should be taken into account for both *in vitro* and *in vivo* determination of bulk tissue optical parameters. © 2003 Optical Society of America

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Within the radiative transfer (RT) theory, the optical response of bulk tissue is modeled with a scattering coefficient μ_s, an absorption coefficient μ_a, and a phase function $p(\mathbf{s}, \mathbf{s}')$ that describes the probability of light being scattered from a direction $\mathbf{s}'$ to direction $\mathbf{s}$. Since analytical solutions of the RT theory cannot be found for nearly all practical cases, modeling of tissue optics often has to be achieved statistically through Monte Carlo (MC) methods.[1–4] For cases in which light distribution is dominated by multiple light scattering, various diffusion approximations of the RT theory have been proposed and investigated for *in vivo* determination of tissue optical parameters.[5] Under these approximations only μ_a and the reduced scattering coefficient $\mu_s' = \mu_s(1 - g)$ are required for modeling, where g is the anisotropy factor defined as the first moment of the phase function.

The bulk parameters cannot be measured directly. An iterative process is often used in which the difference between the measured and the calculated values of light signals is minimized by adjustment of the parameters. The MC methods provide the most accurate model for calculations with the flexibility to simulate the actual configuration of the experiment. The first results obtained with MC modeling for inverse determination of μ_s, μ_a, and g were reported on human breast tissues by measurement of diffuse reflectance R_d, diffuse transmittance T_d, and collimated transmittance T_c.[6] This method was further applied to different tissues[7] and spectral regions[8] and was also modified to determine μ_s and μ_a through the measurement of R_d and T_d by assuming a fixed value for g.[9] Other methods of modeling include the adding–doubling method for slab tissues *in vitro*[10,11] and the diffusion model for the determination of μ_a and μ_s' *in vivo* based on the measurements of spatially resolved reflectance with fiber probes.[5,12] The common element of the reported *in vitro* measurements is the use of thin slab tissue samples with thickness varying from 50 μm to 2 mm, and no one has considered the effects of surface roughness. However, all the tissue sample surfaces possess a certain degree of roughness, and our preliminary measurements of thin slab samples of fresh porcine skin dermis pressed between two glass plates indicated roughness parameters of the order of micrometers. Our previous simulations of light distribution in skin phantoms with rough interfaces proved that even a moderate index mismatch at the rough interfaces can strongly affect the results.[13] In this Letter we show quantitatively the effect of surface roughness with a moderate index mismatch on the inverse determination of bulk parameters.

We adapted an extensively tested MC code for modeling light distribution in rough tissue samples to calculate (R_d, T_d, T_c).[4,8,13] The assembly of a rough tissue slab between glass plates was modeled by a three-layer structure of cylindrical slabs. The profile functions of the two statistically identical rough plate–tissue interfaces were generated numerically through a stationary Gaussian stochastic process characterized by a rms height δ and a transverse correlation length a.[13] We employed the Henyey–Greenstein phase function to describe scattered light distribution in the sample bulk.[14] The simulation began with a photon incident normally on the smooth air–plate interface and then followed its trajectory through the rough plate–tissue interface. Most of the tracked photons transported into the tissue sample and some, if they were not absorbed, exited from the sample and holder plates through the side surfaces or the air–plate interfaces. The photons that emerged from the assembly were registered separately to obtain (R_d, T_d, T_c) according to their positions on the air–plate interfaces and exit directions, as depicted in Fig. 1. Note here that the T_c was defined in our simulations as the portion of incident photons that leaves the integrating sphere through

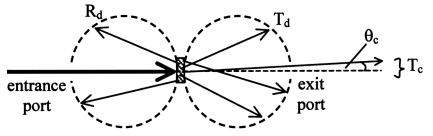

Fig. 1. Definitions of optical signals, with the dashed circles indicating the two positions of the integrating sphere.

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the exit port within a cone angle $\theta_c (= 5.00 \times 10^{-3}$ rad) from the direction of incident light.[6,8] For each configuration of the assembly, we calculated (R_d, T_d, T_c) by using the bulk parameters (μ_a, μ_s, g) and surface parameters (δ, a) with predetermined refractive indices of n_h and n for the sample holder and sample, respectively. To study the effect of surface roughness on inverse determination of optical parameters, we define a square-error function

$$\Sigma = \left(\frac{R_d - R_{d0}}{R_{d0}}\right)^2 + \left(\frac{T_d - T_{d0}}{T_{d0}}\right)^2 + \left(\frac{T_c - T_{c0}}{T_{c0}}\right)^2, \tag{1}$$

where (R_{d0}, T_{d0}, T_{c0}) are either the calculated signals for a reference configuration or the measured signals, and (R_d, T_d, T_c) are those of the investigated configuration. We used Σ as a metric for the iterative process to converge on an optimized set of parameters that stops when $\Sigma \le \Sigma_c$. The value of Σ_c is chosen to be 4×10^{-4}, which corresponds to relative errors of approximately 1% in the measurement of each (R_d, T_d, T_c). The parameter set that needs to be inversely determined can be either of the bulk (μ_s, μ_a, g) or of the surface (δ, a) with the other set treated as known.

We started by investigating first the effect of surface parameters on the inverse determination of bulk parameters. Refractive indices were set to $n = 1.41$ and $n_h = 1.52$ for samples of skin dermis and a glass holder, respectively, near the light wavelength of $\lambda = 1\ \mu$m. It was confirmed that the inverse solution of (μ_s, μ_a, g) can be uniquely determined by minimization of Σ for each different set of surface parameters so that the updated values of (R_d, T_d, T_c) approach the reference values. As an example, we considered a case by use of $\mu_{s0} = 5.00\ \text{mm}^{-1}$, $\mu_{a0} = 0.20\ \text{mm}^{-1}$, $g_0 = 0.900$, $\delta_0 = 10.0\ \mu$m, and $a_0 = 100\ \mu$m for the reference configuration. When the transverse correlation length was changed from the reference value a_0 to $a = 200\ \mu$m with $\delta = \delta_0$, we uniquely determined the bulk parameters to be $\mu_s = 11.3\ \text{mm}^{-1}$, $\mu_a = 0.40\ \text{mm}^{-1}$, and $g = 0.95$ by minimizing Σ in the ranges of $10.0 < \mu_s < 12.0\ \text{mm}^{-1}$, $0.30 < \mu_a < 0.50\ \text{mm}^{-1}$, and $0.90 < g < 1.00$. Furthermore, we found that the relative role of δ and a on the values of bulk parameters can be combined approximately into a single slope factor of δ/a. The effect of surface roughness in terms of δ/a on the inverse determination of bulk parameters is shown in Fig. 2. We note that the data presented in Fig. 2 were obtained for two different cases of $\mu_{s,0}$, corresponding to different optical thicknesses of 1.02 and 3.04 for a 0.2-mm-thick sample, with the reference configurations for both cases of $\delta/a = 0.10$ ($a_0 = 100\ \mu$m, $\delta_0 = 10\ \mu$m).

As shown in Fig. 2 the effect of surface roughness is significant on the inverse determination of the bulk parameters of μ_s, μ_a, and g. This is especially the case for samples of small optical thicknesses: μ_s decreases from approximately 22 to 1 mm^{-1} and μ_a from 0.55 to 0.1 mm^{-1} when the slope factor δ/a varies between 0.01 and 0.20. The change in $\mu_s(\mu_a)$ can be understood since the scattering (absorption) coefficient is defined as the probability of photons being scattered (absorbed) per unit of path length. For rough samples, more photons are deflected out of the original path at the surfaces than smooth samples. To keep the updated values of R_d and T_d close to the reference, μ_s has to be reduced for rough samples. As a result, the average path length of tracked photons within the rough sample is increased and μ_a has to be reduced as well to keep the portion of absorbed photons the same as the reference configuration. Anisotropy factor g was found to decrease significantly as the surface of the tissue sample become rough. Thus it was shown that a moderate index mismatch of $\Delta n = 0.11$ can severely distort the angular distribution of the light signals. Although the effects of roughness on μ_s, μ_a, and g are similar for both samples of different optical thicknesses, the responses of μ_s' to the roughness are profoundly different. As demonstrated by the insets in Figs. 2(c) and 2(f), μ_s' for the optical thick sample is insensitive to the roughness and μ_s' of the optical thin sample changes with roughness similar to that of μ_s, indicating that in the single-scattering or nondiffusive regime light signals are significantly affected by the surface roughness. These results strongly suggest that the effect of surface roughness needs to be carefully analyzed for *in vivo* determination of bulk tissue optical parameters from the reflectance measurements, where the nondiffusive regime dominates the light remitted from the superficial layer of the tissue near the light source.

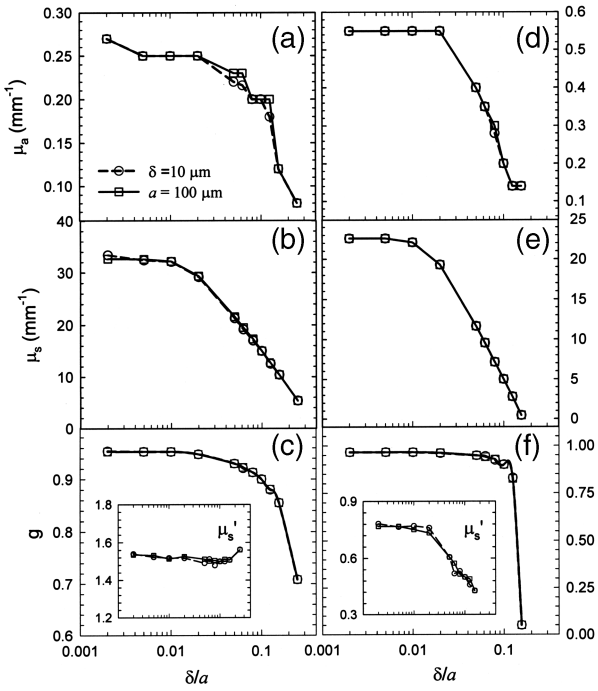

Fig. 2. Dependence of μ_a, μ_s, and g on δ/a. The bulk parameters of the sample for the reference configuration are $\mu_{a0} = 0.2\ \text{mm}^{-1}$ and $g_0 = 0.90$; (a)–(c), $\mu_{s0} = 15\ \text{mm}^{-1}$; (d)–(f), $\mu_{s0} = 5\ \text{mm}^{-1}$. Other parameters are 0.20-mm, 14-mm diameter, $n = 1.41$ for the sample, and 3 mm, 22 mm, and 1.51 for the holder plates, respectively. Insets in (c) and (f) indicate μ_s' as functions of δ/a. Two groups of data are compared in each figure with either δ or a kept as a constant. The solid curves are to guide the eye.

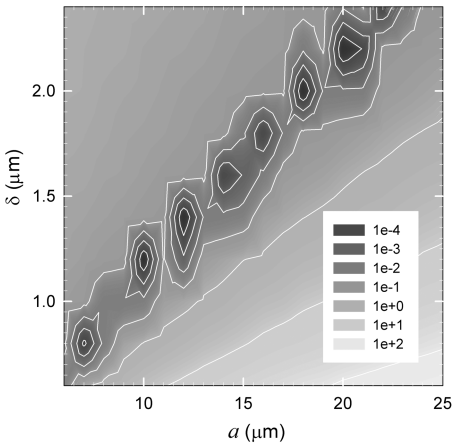

Fig. 3. Contour plot of error function Σ versus surface parameters δ and a for the Intralipid sample between rough windows.

To verify our numerical results, we measured T_d, T_c, and R_d of Intralipid samples between two 3-mm-thick BK7 windows (WNL0103, Casix). One pair of windows was made rough on one side with Al_2O_3 particles of nominal 9.5-μm size (optical polishing powder, Universal Photonics). We diluted an Intralipid-20% solution (Baxter Healthcare) with deionized water by a ratio of 1:7 to obtain samples of $\mu_s \approx 15\ \mathrm{mm}^{-1}$.[14] The refractive index of the Intralipid sample n_s was determined to be 1.34 at $\lambda = 633$ nm by use of a refractometer built for turbid samples. Optical measurements of the identical Intralipid samples in two pairs of windows, smooth and rough, were carried out with a laser beam of $\lambda = 633$ nm, modulated at 17 Hz and detected with a Si photodiode and a lock-in amplifier. The T_d and R_d were measured with an integrating sphere and T_c was measured with a spatial filtering setup within the cone angle θ_c as shown in Fig. 1.[8] For the sample between the smooth windows, we obtained $T_d = 32.5\%$, $R_d = 8.44\%$, and $T_c = 4.16\%$ for a 0.20-mm-thick sample, and these were used as the reference values in Eq. (1) to determine the bulk parameters of the Intralipid samples by assuming that $\delta = 0$. This produced $\mu_s = 14.0\ \mathrm{mm}^{-1}$, $\mu_a = 0.94\ \mathrm{mm}^{-1}$, and $g = 0.76$. For the sample between rough windows, the measured values changed to $T_d = 32.4\%$, $R_d = 9.23\%$, and $T_c = 0.038\%$ for the same thickness, and they were used as the reference values to determine possible values of surface parameters by calculating Σ as a function of δ and a. Identical bulk parameters of μ_s, μ_a, and g were used as the input parameters since the Intralipid samples were identical. The results are plotted in Fig. 3, which clearly demonstrates that δ and a cannot be uniquely determined in this process except for the ratio $\delta/a(\approx 0.11)$. We also determined the bulk parameters from measured T_d, T_c, and R_d by neglecting surface roughness with $\delta = 0$ and found that they became $\mu_s = 38.8\ \mathrm{mm}^{-1}$, $\mu_a = 1.3\ \mathrm{mm}^{-1}$, and $g = 0.89$. These results agree with the data in Fig. 2.

In summary we have developed a MC model-based inverse process to extract bulk optical parameters from light signals measured from tissue samples with surface roughness on scales close to the wavelength of light. It has been shown clearly that the surface roughness can significantly affect the values of bulk tissue optical parameters (including μ_a) inversely determined from *in vitro* and *in vivo* studies even for a moderate index mismatch.

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