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Abstract: We investigate methods of linearizing the problem of diffuse reflectance spectroscopy. Simulations show the effective optical pathlength varying in a scattering medium as a function of wavelength, total absorption, and chosen polarization channels.

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1. Introduction

Spectrometry involves the analysis of chromophore content by observing the wavelength dependent attenuation of light which has propagated through a sample. Some knowledge of the pathlength through which light has travelled is needed to treat this problem. Typically, instruments involving the transmission geometry are favoured, as this path is predictable. However, in the presence of scattering, the optical pathlength depends non-trivially on the wavelength, and on the total level of absorption. As a result, the relationship between the measured attentuation, and the medium absorption, becomes non-linear. Previous work [1] has employed polarization filtering in an attempt to linearize this problem in the transmission geometry, as polarization maintaining photons are more likely to follow direct paths along the transmission axis [2]. This allows simple models, such as the modified Beer-Lambert law to still be applied to this problem effectively. We are interested in solving this problem in the reflectance (backscattering) geometry, using wide field illumination, and wide field detection. This geometry is relevant to applications which seek to characterize the spatial distribution of numerous chromophores in a rapid, and non-invasive manner. Here, we investigate the potential use of linear, elliptical, and circular polarization filtering in an analogous manner to [1], in order to maintain a constant effective optical pathlength between measurements made at different wavelengths. These different forms of polarization have previously been observed to experience quite different transport within scattering media [3], suggesting that they may offer some control over the optical path. Furthermore, if a constant pathlength can be achieved through polarization modulation, then consistency of the probing volume will also likely improve, reducing errors incurred by mesoscopic inhomogeneities in the medium under investigation.

2. The modified Beer-Lambert law

The simplified linear model of attenuation we wish to apply to diffuse reflectance spectroscopy, is the modified Beer-Lambert law. In Brief, for a medium containing N-number of chromophores, each with absorption spectra given by $\varepsilon_i(\lambda)$, the attenuation of a source of incident intensity $I_0(\lambda)$, can be represented as [1]:

$$A(\lambda) = \log\left(\frac{I_0(\lambda)}{I(\lambda)}\right) = A_s + \left(\sum_{i=1}^{N} \varepsilon_i(\lambda)\rho_i\right)\ell\,, \tag{1}$$

where $I(\lambda)$ is the measured intensity, A_s is the attenuation due to scattering, ℓ is the 'effective pathlength', and ρ_i, is the concentration of the i-th chromophore. In cases where the above equation is applicable, continuous wave measurements are only capable of recovering the relative concentrations of the chromophores, and require the attenuation to be measured at $N+1$ wavelengths [1]. Note that in this formulation, both the attenuation due to scattering, A_s, and the effective pathlength ℓ are assumed to be wavelength independent. This is a particularly poor assumption in the backscattering geometry, which we look to remedy by applying a wavelength dependent correction in the form of varying polarization channels.

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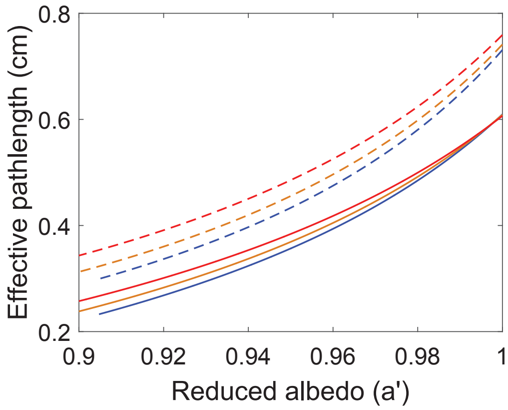

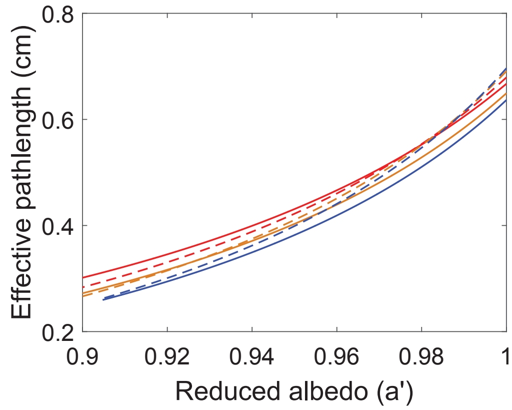

Fig. 1. (a) Effective pathlength as a function of the reduced scattering albedo for co-linear (solid), and cross-linear (dashed) channels. 532nm, 570nm, and 633nm wavelengths are represented as blue, orange, and red lines, respectively. (b) Effective pathlength as a function of the reduced scattering albedo for co-circular (solid), and cross-circular (dashed) channels.

3. Wavelength and polarization dependence of the effective pathlength

In order to assess the wavelength and polarization dependence of the effective optical pathlength in the backscattering geometry, we employed Monte Carlo simulations using medium properties that approximate an Intralipid based scattering medium (Such that we can later compare to experiment in a controlled manner). The single scattering matrix used in the simulations was generated using Mie theory, with an exponential distribution of spherical particles similar to that found in [4]. Simulations were carried out at three wavelengths of interest (which each required a new single scattering matrix to be calculated), namely, $\lambda_1 = 532$nm, $\lambda_2 = 570$nm, $\lambda_3 =$ and 633nm. Attenuation measurements made at this number of wavelengths would allow the recovery of the ratio of concentrations of two chromophore species in a case where Eq. (1) could be applied. The scattering asymmetry parameter of the medium was $g = 0.75$, at 633nm. For each wavelength, the total backscattered reflectance from a slab was calculated for different values of the reduced scattering albedo, $a' = \mu_s'/(\mu_a + \mu_s')$, over the range $0.9 \leq a' \leq 1.0$. Normalizing each measured value of the reflectance to that of the case where $a' = 1.0$, allows for the scattering attenuation term, A_s, to be removed from Eq. (1). Then, taking the differential of the simulated attenuation relative to the absorption coefficient, μ_a, produces the effective pathlength, which can be represented as a function of the reduced albedo of the medium for each wavelength, $\ell(a', \lambda)$. These same simulations were repeated, using different polarization channels (different combinations of input polarization, and filtering upon detection). It was observed (see Fig. 1) that the effective pathlength changes depending on the polarization channel selected. The most clearly observed difference was between co-linear and cross-linear channels (Fig. 1(a)). As expected, co-linear has the shortest effective pathlength, as this channel is dominated by light which scatters only superficially, largely maintaining it's polarization. The cross-linear signal on the other hand, results largely from depolarized light, which has typically propagated further. The unpolarized channel (not shown here) fell intermediate to these two extremes. Also, the co-circular, and cross-circular channels demonstrated an interesting variation of pathlength, with each exhibiting a crossover at some value of the reduced albedo (Fig. 1(b)). The pathlength of various elliptical channels (not shown here), also fell in the intermediate range between the co-linear, and cross-linear channels.

From the above observations, it appears that at least over a certain range, the variation in the effective pathlength caused by a change in wavelength (both due to the changing scattering properties, and the implicit change in the albedo), is comparable to the variation in pathlength caused by changing the polarization imaging channel. This suggests that if the effect of changing polarization is well understood for a given medium, then this could be used to counter the effects of wavelength induced changes to the pathlength, thus maintaining a near-constant path over the wavelength range used, and improving the accuracy of chromophore information gathered using Equation (1).

4. Conclusions

Here we have demonstrated the potential for polarization filtering to enable a simple linear model of attenuation in the backscattering geometry, for employment in spatially resolved diffuse reflectance spectroscopy. Polarization filtering was demonstrated to alter the effective optical pathlength in a scattering medium, and with a magnitude that is comparable to that which occurs by varying the radiation wavelength. We suggest that if a suitable polarization channel is selected at each wavelength, then the optical pathlength could potentially remain near-constant, allowing the modified Beer-Lambert law to be applied. We note that for this method to be carried out practically, knowledge of the reduced scattering albedo $a'(\lambda)$ of the medium under investigation, may need to be provided. Investigations are currently in progress to demonstrate this application experimentally, using solutions of Intralipid and optical dyes.

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