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Subdiffuse scattering and absorption model for single fiber reflectance spectroscopy: supplement

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Supplemental materials

Here we will demonstrate that the diffuse contribution to the SFR signal can be rewritten as a function of μ_s 'd and μ_p/μ_s '. The diffuse reflectance per unit area as a function of radial coordinate ρ is given by Farrell *et al* as [1]:

$$
R(\rho) = \frac{a'}{4\pi} \left(z_0 \left[\mu_{eff} + \frac{1}{r_1} \right] \frac{e^{-\mu_{eff}r_1}}{r_1^2} + (z_0 + 2z_b) \left[\mu_{eff} + \frac{1}{r_2} \right] \frac{e^{-\mu_{eff}r_2}}{r_2^2} \right)
$$
(S1)

where $a' = \mu_s / (\mu_s' + \mu_a)$ and μ_{eff} is the effective attenuation coefficient, $\mu_{eff} = \sqrt{\mu_a/D}$ $\sqrt{3\mu_a\mu_s'}$. The position of the point source in the medium is set at one reduced mean free path given by $z_0 = 1/\mu_s$. The location of the 'virtual boundary', where the fluence rate has to be zero, is given by $z_b = 2AD$ where A is a parameter that depends on the refractive index mismatch between the fiber and the tissue [2]. We can express equation S1 in terms of dimensionless variables $x = \mu_s d$, $y = \mu_a/\mu_s$ and $\beta = \rho/d$. We also use the constant $c_A = 1 +$ $4A/3$ to compact the expression. Using these substitutions, the distances r_1 and r_2 are:

$$
r_1^2 = z_0^2 + \rho^2 = \left(\frac{d}{x}\right)^2 + d^2 \cdot \beta^2 = \frac{d^2}{x^2} (1 + x^2 \beta^2)
$$
 (S2)

$$
r_2^2 = (z_0 + 2z_b)^2 + \rho^2 = \left(\frac{d}{x} + \frac{4A \cdot d}{3x}\right)^2 + d^2 \cdot \beta^2 = \frac{d^2}{x^2} \left(\left(1 + \frac{4A}{3}\right)^2 + x^2 \beta^2\right) \tag{S3}
$$

and

$$
\frac{d^2}{dx^2} \cdot R(y, x\beta) = \frac{(1+y)^{-1}}{4\pi} \left[\left(\frac{\sqrt{3y}}{1 + (x\beta)^2} + \frac{1}{(1 + (x\beta)^2)^{\frac{3}{2}}} \right) e^{-\sqrt{3y(1 + (x\beta)^2)}} + c_A \left(\frac{\sqrt{3y}}{c_A^2 + (x\beta)^2} + \frac{1}{(c_A^2 + (x\beta)^2)^{\frac{3}{2}}} \right) e^{-\sqrt{3y(c_A^2 + (x\beta)^2)}} \right]
$$
(S4)

Likewise, the probability distribution for distances on the fiber surface:

$$
p(\rho) = \frac{16\rho}{\pi d^2} \cos^{-1} \left(\frac{\rho}{d}\right) - \frac{16}{\pi d} \left(\frac{\rho}{d}\right)^2 \sqrt{1 - \left(\frac{\rho}{d}\right)^2} \tag{S5}
$$

can be rewritten as:

$$
d \cdot p(\beta) = \left(\frac{16}{\pi} \beta \cos^{-1}(\beta) - \frac{16}{\pi} \beta^2 \sqrt{1 - \beta^2}\right)
$$
 (S6)

Such that the integrated reflectance

$$
R_{dif} = \frac{\pi}{4} \cdot d^2 \cdot \int_0^d R(\rho) \cdot p(\rho, d) d\rho \tag{S7}
$$

Is rewritten as:

$$
R_{dif}(x,y) = \frac{\pi}{4} \cdot x^2 \cdot \int_0^1 R(y,\beta x) \cdot p(\beta) d\beta
$$
 (S8)

For the integration in this form with integration variable β ; the factors x and y are simply constants that are carried over. Consequently, in the resulting expression the absorption coefficient will appear in the ratio μ_a/μ_s , and the fiber diameter will appear in the product $\mu_s'd.$

References

- T. J. Farrell, M. S. Patterson, and B. Wilson, "A diffusion theory model of spatially resolved, steady-state diffuse reflectance for the noninvasive determination of tissue optical properties in vivo," Med. Phys. 19, 879–8 $1.$
- $\overline{2}$.