Supplemental Document

Biomedical Optics EXPRESS

Theoretical investigation of photon partial pathlengths in multilayered turbid media: supplement

HÉCTOR A. GARCÍA,* DEMIÁN A. VERA, MARÍA. V. WAKS SERRA, GUIDO R. BAEZ, DANIELA I. IRIARTE, AND JUAN A. POMARICO

CIFICEN (UNCPBA-CONICET-CICPBA), Pinto 399, B7000GHG Tandil, Argentina
**hgarcia@exa.unicen.edu.ar*

Supplement DOI: https://doi.org/10.6084/m9.figshare.19121702

Parent Article DOI: https://doi.org/10.1364/BOE.449514

Theoretical investigation of photons partial pathlengths in multilayered turbid media: supplemental document

In this supplementary material we introduce the needed expressions to compute the mean partial pathlengths (MPPLs) of photons in three- and four-layered media, according to the details shown in the accompanying paper.

THREE AND FOUR-LAYERED MEDIA MEAN PARTIAL PATHLENGTHS

Three-layered media

Following the reasoning described in Section 2 of the manuscript, for three-layered media the computation of analytical expressions of $R(\rho)$ and, thus, of the MPPLs, require the use of β_N and γ_N and their derivatives with respect to $\mu_{a,i}$:

$$\beta_3 = D_2\alpha_2 n_2^2 \cosh(\alpha_2 l_2) + D_3\alpha_3 n_3^2 \sinh(\alpha_2 l_2) \tag{S1}$$

$$\gamma_3 = D_2\alpha_2 n_2^2 \sinh(\alpha_2 l_2) + D_3\alpha_3 n_3^2 \cosh(\alpha_2 l_2). \tag{S2}$$

From these expressions we obtain:

$$\frac{\partial\beta_3}{\partial\alpha_2}\frac{\partial\alpha_2}{\partial\mu_{a,2}} = \left\{D_2 n_2^2\left[\cosh(\alpha_2 l_2) + \alpha_2 l_2 \sinh(\alpha_2 l_2)\right] + D_3 n_3^2 \alpha_3 l_2 \cosh(\alpha_2 l_2)\right\}\frac{\partial\alpha_2}{\partial\mu_{a,2}}, \tag{S3}$$

$$\frac{\partial\gamma_3}{\partial\alpha_2}\frac{\partial\alpha_2}{\partial\mu_{a,2}} = \left\{D_2 n_2^2\left[\sinh(\alpha_2 l_2) + \alpha_2 l_2 \cosh(\alpha_2 l_2)\right] + D_3 n_3^2 \alpha_3 l_2 \sinh(\alpha_2 l_2)\right\}\frac{\partial\alpha_2}{\partial\mu_{a,2}}, \tag{S4}$$

$$\frac{\partial\beta_3}{\partial\alpha_3}\frac{\partial\alpha_3}{\partial\mu_{a,3}} = D_3 n_3^2 \sinh(\alpha_2 l_2)\frac{\partial\alpha_3}{\partial\mu_{a,3}}, \tag{S5}$$

$$\frac{\partial\gamma_3}{\partial\alpha_3}\frac{\partial\alpha_3}{\partial\mu_{a,3}} = D_3 n_3^2 \cosh(\alpha_2 l_2)\frac{\partial\alpha_3}{\partial\mu_{a,3}}; \tag{S6}$$

with:

$$\frac{\partial\alpha_2}{\partial\mu_{a,2}} = \frac{1}{2D_2\alpha_2}, \tag{S7}$$

$$\frac{\partial\alpha_3}{\partial\mu_{a,3}} = \frac{1}{2D_3\alpha_3}. \tag{S8}$$

We refer again to Eqs. (12-16), where the Green's function is written as:

$$G_1(\alpha_1,\alpha_2) = \mathcal{A}(\alpha_1) + \mathcal{B}(\alpha_1)\mathcal{C}(\alpha_1,\alpha_2), \tag{S9}$$

and separated as:

$$\mathcal{A}(\alpha_1) = \frac{e^{-\alpha_1 z_0} - e^{-\alpha_1(z_0+2z_{b,1})}}{2\alpha_1 D_1}, \tag{S10}$$

$$\mathcal{B}(\alpha_1) = \frac{\sinh\left[\alpha_1(z_0+z_{b,1})\right]\sinh(\alpha_1 z_{b,1})}{D_1\alpha_1 e^{\alpha_1(l_1+z_{b,1})}}, \tag{S11}$$

$$\mathcal{C}(\alpha_1,\alpha_2,\alpha_3) = \frac{D_1\alpha_1 n_1^2\beta_3 - D_2\alpha_2 n_2^2\gamma_3}{D_1\alpha_1 n_1^2\beta_3\cosh\left[\alpha_1(l_1+z_{b,1})\right] + D_2\alpha_2 n_2^2\gamma_3\sinh\left[\alpha_1(l_1+z_{b,1})\right]}. \tag{S12}$$

Thus, the derivatives of the Green's function are:

$$\frac{\partial G_1}{\partial \alpha_1}\frac{\partial \alpha_1}{\partial \mu_{a,1}} = \left(\frac{\partial \mathcal{A}}{\partial \alpha_1} + \frac{\partial \mathcal{B}}{\partial \alpha_1}\mathcal{C} + \frac{\partial \mathcal{C}}{\partial \alpha_1}\mathcal{B}\right)\frac{\partial \alpha_1}{\mu_{a,1}} \tag{S13}$$

$$\frac{\partial G_1}{\partial \alpha_2}\frac{\partial \alpha_2}{\partial \mu_{a,2}} = \frac{\partial \mathcal{C}}{\partial \alpha_2}\frac{\partial \alpha_2}{\partial \mu_{a,2}} \cdot \mathcal{B} \tag{S14}$$

$$\frac{\partial G_1}{\partial \alpha_3}\frac{\partial \alpha_3}{\partial \mu_{a,3}} = \frac{\partial \mathcal{C}}{\partial \alpha_3}\frac{\partial \alpha_3}{\partial \mu_{a,3}} \cdot \mathcal{B}. \tag{S15}$$

We use the notation:

$$\delta = D_1 n_1^2 \alpha_1 \beta_3 - D_2 n_2^2 \alpha_2 \gamma_3, \tag{S16}$$

$$\Delta = D_1 n_1^2 \alpha_1 \beta_3 \cosh\left[\alpha_1 (l_1 + z_{b,1})\right] - D_2 n_2^2 \alpha_2 \gamma_3 \sinh\left[\alpha_1 (l_1 + z_{b,1})\right], \tag{S17}$$

so the term $\mathcal{C}$ becomes:

$$\mathcal{C} = \frac{\delta}{\Delta} \Rightarrow \frac{\partial \mathcal{C}}{\partial \alpha_i} = \left(\frac{\partial \delta}{\partial \alpha_i} \cdot \Delta - \frac{\partial \Delta}{\partial \alpha_i} \cdot \delta\right) \cdot \Delta^{-2}. \tag{S18}$$

From now on, we will use Eq. (S18) in terms of δ and Δ to compute $\mathcal{C}$ and its derivatives. Next, from expression Eq. (S13) we have:

$$\frac{\partial \mathcal{A}}{\partial \alpha_1} = \frac{e^{-\alpha_1 z_0}}{2 D_1 \alpha_1^2}\left[\alpha_1 \left(z_0 + 2 z_{b,1}\right) e^{-2 z_{b,1}} - \alpha_1 z_0 - 1\right]. \tag{S19}$$

$$\frac{\partial \mathcal{B}}{\partial \alpha_1} = \frac{e^{-\alpha_1 (l_1 + z_{b,1})}}{D_1 \alpha_1}\Big(\left\{ (z_0 + z_{b,1}) \cosh\left[\alpha_1 (z_0 + z_{b,1})\right] \sinh\left(\alpha_1 z_{b,1}\right) + z_{b,1} \sinh[\alpha_1 (z_0 + z_{b,1})] \cosh\left(\alpha_1 z_{b,1}\right) \right\} \alpha_1 - \sinh\left[\alpha_1 (z_0 + z_{b,1})\right] \sinh\left(\alpha_1 z_{b,1}\right) [1 + \alpha_1 (l_1 + z_{b,1})] \Big). \tag{S20}$$

And, referring to Eq. (S18):

$$\frac{\partial \delta}{\partial \alpha_1} = D_1 n_1^2 \beta_3. \tag{S21}$$

$$\frac{\partial \Delta}{\partial \alpha_1} = \left[D_1 n_1^2 \beta_3 + D_2 n_2^2 \alpha_2 \gamma_3 (l_1 + z_{b,1})\right] \cosh\left[\alpha_1 (l_1 + z_{b,1})\right] + \tag{S22}$$

$$D_1 n_1^2 \beta_3 \alpha_1 \sinh\left[\alpha_1 (l_1 + z_{b,1})\right] (l_1 + z_{b,1}). \tag{S23}$$

And, for L_2 and L_3:

$$\frac{\partial \delta}{\partial \alpha_2} = D_1 n_1^2 \alpha_1 \beta_{3,2} - D_2 n_2^2 (\gamma_3 + \alpha_2 \gamma_{3,2}), \tag{S24}$$

$$\frac{\partial \Delta}{\partial \alpha_2} = D_1 n_1^2 \alpha_1 \cosh\left[\alpha_1 (l_1 + z_{b,1})\right] \beta_{3,2} + D_2 n_2^2 \sinh\left[\alpha_1 (l_1 + z_{b,1})\right] \left[\gamma_{3,2} \alpha_2 + \gamma_3\right], \tag{S25}$$

$$\frac{\partial \delta}{\partial \alpha_3} = D_1 n_1^2 \alpha_1 \beta_{3,3} - D_2 n_2^2 \alpha_2 \gamma_{3,3}, \tag{S26}$$

$$\frac{\partial \Delta}{\partial \alpha_3} = D_1 n_1^2 \alpha_1 \beta_{3,3} \cosh\left[\alpha_1 (l_1 + z_{b,1})\right] - D_2 n_2^2 \alpha_2 \gamma_{3,3} \sinh\left[\alpha_1 (l_1 + z_{b,1})\right]. \tag{S27}$$

(S28)

Here:

$$\beta_{3,j} = \frac{\partial \beta_3}{\partial \alpha_j}, \qquad \gamma_{3,j} = \frac{\partial \gamma_3}{\partial \alpha_j}, \tag{S29}$$

Expressions from Eq. (S1) to Eq. (S29) are used in:

$$\frac{\partial R}{\partial \mu_{a,j}} = \frac{1}{4 A_n \pi^2 R_{\mathrm{EB}}^2} \sum_{n=1}^{\infty} \left[\frac{\partial G_1(\boldsymbol{\alpha})}{\partial \mu a, j} \frac{J_0(s_n \rho)}{J_1^2(s_n R_{\mathrm{EB}})}\right]. \tag{S30}$$

This quantities, in combination with R(ρ), can be used to compute L_1, L_2 and L_3:

$$L_j(\lambda,\rho) = -\frac{1}{R(\rho)}\frac{\partial R(\rho)}{\partial \mu_{a,j}(\lambda)}. \tag{S31}$$

Thus:

$$\begin{aligned} L_1 = &-\frac{1}{R(\rho)} \times \frac{1}{4A_n\pi^2 R_{\text{EB}}^2}\sum_{n=1}^{\infty}\Bigg\{\frac{e^{-\alpha_1 z_0}}{2D_1\alpha_1^2}\Big[\alpha_1\left(z_0+2z_{b,1}\right)e^{-2z_{b,1}}-\alpha_1 z_0-1\Big]+ \\ &\frac{e^{-\alpha_1(l_1+z_{b,1})}}{D_1\alpha_1}\Bigg(\Big\{(z_0+z_{b,1})\cosh\left[\alpha_1(z_0+z_{b,1})\right]\sinh\left(\alpha_1 z_{b,1}\right)+z_{b,1}\sinh[\alpha_1(z_0+ \\ &z_{b,1})]\cosh\left(\alpha_1 z_{b,1}\right)\Big\}\alpha_1-\sinh\left[\alpha_1(z_0+z_{b,1})\right]\sinh\left(\alpha_1 z_{b,1}\right)[1+\alpha_1(l_1+z_{b,1})]\Bigg)\times\frac{\delta}{\Delta}+ \\ &\left(\frac{\partial\delta}{\partial\alpha_1}\cdot\Delta-\frac{\partial\Delta}{\partial\alpha_1}\cdot\delta\right)\cdot\Delta^{-2}\times\frac{\sinh\left[\alpha_1(z_0+z_{b,1})\right]\sinh\left(\alpha_1 z_{b,1}\right)}{D_1\alpha_1 e^{\alpha_1(l_1+z_{b,1})}}\Bigg\}, \end{aligned} \tag{S32}$$

$$L_2 = -\frac{1}{R(\rho)} \times \frac{1}{4A_n\pi^2 R_{\text{EB}}^2}\sum_{n=1}^{\infty}\left\{\left(\frac{\partial\delta}{\partial\alpha_1}\cdot\Delta-\frac{\partial\Delta}{\partial\alpha_2}\cdot\delta\right)\cdot\Delta^{-2}\times\frac{\sinh\left[\alpha_2(z_0+z_{b,1})\right]\sinh\left(\alpha_1 z_{b,1}\right)}{D_1\alpha_1 e^{\alpha_1(l_1+z_{b,1})}}\right\}, \tag{S33}$$

$$L_3 = -\frac{1}{R(\rho)} \times \frac{1}{4A_n\pi^2 R_{\text{EB}}^2}\sum_{n=1}^{\infty}\left\{\left(\frac{\partial\delta}{\partial\alpha_1}\cdot\Delta-\frac{\partial\Delta}{\partial\alpha_2}\cdot\delta\right)\cdot\Delta^{-2}\times\frac{\sinh\left[\alpha_3(z_0+z_{b,1})\right]\sinh\left(\alpha_3 z_{b,1}\right)}{D_1\alpha_1 e^{\alpha_1(l_1+z_{b,1})}}\right\}. \tag{S34}$$

Four-layered media

The procedure for finding the mean partial pathlengths of a four-layered media is quite similar to that described in the previous section. The main difference is the dependence of $\mathcal{C}$ with $\mu_{a,4}$ through the parameter α_4:

$$\mathcal{C}(\alpha_1,\alpha_2,\alpha_3,\alpha_4) = \frac{D_1\alpha_1 n_1^2\beta_3 - D_2\alpha_2 n_2^2\gamma_3}{D_1\alpha_1 n_1^2\beta_3\cosh\left[\alpha_1(l_1+z_{b,1})\right]+D_2\alpha_2 n_2^2\gamma_3\sinh\left[\alpha_1(l_1+z_{b,1})\right]}. \tag{S35}$$

Now, the factors β and γ, which have the form:

$$\beta_3 = D_2\alpha_2 n_2^2\beta_4\cosh\left(\alpha_2 l_2\right)+D_3\alpha_3 n_3^2\gamma_4\sinh\left(\alpha_2 l_2\right), \tag{S36}$$

$$\gamma_3 = D_2\alpha_2 n_2^2\beta_4\sinh\left(\alpha_2 l_2\right)+D_3\alpha_3 n_3^2\gamma_4\cosh\left(\alpha_2 l_2\right), \tag{S37}$$

$$\beta_4 = D_3 n_3^2\alpha_3\cosh\left(\alpha_3 l_3\right)+D_4 n_4^2\alpha_4\sinh\left(\alpha_3 l_3\right), \tag{S38}$$

$$\gamma_4 = D_3 n_3^2\alpha_3\sinh\left(\alpha_3 l_3\right)+D_4 n_4^2\alpha_4\cosh\left(\alpha_3 l_3\right), \tag{S39}$$

are needed. From these expressions, their derivatives are easily obtained:

$$\frac{\partial \beta_3}{\partial \alpha_2}\frac{\partial \alpha_2}{\mu_{a,2}} = \left\{D_2 n_2^2 \beta_4 \left[\cosh\left(\alpha_2 l_2\right) + \alpha_2 l_2 \sinh\left(\alpha_2 l_2\right)\right] + D_3 n_3^2 \alpha_3 \gamma_4 l_2 \cosh\left(\alpha_2 l_2\right)\right\} \frac{\partial \alpha_2}{\partial \mu_{a,2}}. \tag{S40}$$

$$\frac{\partial \gamma_3}{\partial \alpha_2}\frac{\partial \alpha_2}{\mu_{a,2}} = \left\{D_2 n_2^2 \beta_4 \left[\sinh\left(\alpha_2 l_2\right) + \alpha_2 l_2 \cosh\left(\alpha_2 l_2\right)\right] + D_3 n_3^2 \alpha_3 \gamma_4 l_2 \sinh\left(\alpha_2 l_2\right)\right\} \frac{\partial \alpha_2}{\partial \mu_{a,2}}. \tag{S41}$$

$$\frac{\partial \beta_3}{\partial \alpha_3}\frac{\partial \alpha_3}{\mu_{a,3}} = \left[D_2 n_2^2 \alpha_2 \beta_{4,3} \cosh\left(\alpha_2 l_2\right) + D_3 n_3^2 \sinh\left(\alpha_2 l_2\right)\left(\gamma_4 + \alpha_3 \gamma_{4,3}\right)\right] \frac{\partial \alpha_3}{\partial \mu_{a,3}}. \tag{S42}$$

$$\frac{\partial \gamma_3}{\partial \alpha_3}\frac{\partial \alpha_3}{\mu_{a,3}} = \left[D_2 n_2^2 \alpha_2 \beta_{4,3} \sinh\left(\alpha_2 l_2\right) + D_3 n_3^2 \cosh\left(\alpha_2 l_2\right)\left(\gamma_4 + \alpha_3 \gamma_{4,3}\right)\right] \frac{\partial \alpha_3}{\partial \mu_{a,3}}. \tag{S43}$$

$$\frac{\partial \beta_4}{\partial \alpha_3}\frac{\partial \alpha_3}{\mu_{a,3}} = \left\{D_3 n_3^2 \left[\cosh\left(\alpha_3 l_3\right) + \alpha_3 l_3 \sinh\left(\alpha_3 l_3\right)\right] + D_4 n_4^2 \alpha_4 l_3 \cosh\left(\alpha_3 l_3\right)\right\} \frac{\partial \alpha_3}{\partial \mu_{a,3}} \tag{S44}$$

$$\frac{\partial \gamma_4}{\partial \alpha_3}\frac{\partial \alpha_3}{\mu_{a,3}} = \left\{D_3 n_3^2 \left[\sinh\left(\alpha_3 l_3\right) + \alpha_3 l_3 \cosh\left(\alpha_3 l_3\right)\right] + D_4 n_4^2 \alpha_4 l_3 \sinh\left(\alpha_3 l_3\right)\right\} \frac{\partial \alpha_3}{\partial \mu_{a,3}}. \tag{S45}$$

$$\frac{\partial \beta_4}{\partial \mu_{a,4}} = D_4 n_4^2 \cosh\left(\alpha_3 l_3\right) \frac{\partial \alpha_4}{\partial \mu_{a,4}} \tag{S46}$$

$$\frac{\partial \gamma_4}{\partial \mu_{a,3}} = D_4 n_4^2 \cosh\left(\alpha_3 l_3\right) \frac{\partial \alpha_4}{\partial \mu_{a,4}}. \tag{S47}$$

Here, we have used relations which are analogous to Eq. (S29) for $\beta_{4,3}$, $\gamma_{4,3}$, $\beta_{3,3}$ and $\gamma_{3,3}$. With all these derivatives, we can refer again to the following formula:

$$\frac{\partial G_1(\boldsymbol{\alpha})}{\partial \mu_{a,j}} = \left(\frac{\partial \mathcal{A}}{\partial \alpha_j} + \frac{\partial \mathcal{B}}{\partial \alpha_j}\mathcal{C} + \mathcal{B}\frac{\partial \mathcal{C}}{\partial \alpha_j}\right)\frac{\partial \alpha_j}{\partial \mu_{a,j}}, \tag{S48}$$

that has to be used entirely to calculate L_1. The only term that does not vanish for L_2, L_3 and L_4 is $\mathcal{B}\frac{\partial \mathcal{C}}{\partial \alpha_j}$, thus:

$$\frac{\partial G_1}{\partial \alpha_1}\frac{\partial \alpha_1}{\partial \mu_{a,1}} = \left(\frac{\partial \mathcal{A}}{\partial \alpha_1} + \frac{\partial \mathcal{B}}{\partial \alpha_1}\mathcal{C} + \frac{\partial \mathcal{C}}{\partial \alpha_1}\mathcal{B}\right)\frac{\partial \alpha_1}{\mu_{a,1}} \tag{S49}$$

$$\frac{\partial G_1}{\partial \alpha_2}\frac{\partial \alpha_2}{\partial \mu_{a,2}} = \frac{\partial \mathcal{C}}{\partial \alpha_2}\frac{\partial \alpha_2}{\partial \mu_{a,2}} \cdot \mathcal{B} \tag{S50}$$

$$\frac{\partial G_1}{\partial \alpha_3}\frac{\partial \alpha_3}{\partial \mu_{a,3}} = \frac{\partial \mathcal{C}}{\partial \alpha_3}\frac{\partial \alpha_3}{\partial \mu_{a,3}} \cdot \mathcal{B}. \tag{S51}$$

$$\frac{\partial G_1}{\partial \alpha_4}\frac{\partial \alpha_4}{\partial \mu_{a,4}} = \frac{\partial \mathcal{C}}{\partial \alpha_4}\frac{\partial \alpha_4}{\partial \mu_{a,4}} \cdot \mathcal{B}. \tag{S52}$$

The remaining procedure, i.e. the definitions of L_i is straightforward and identical to that described in the previous section.