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Heuristic absorption calculation in bilayered media from a white Monte Carlo dataset

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Monte Carlo (MC) simulations can adequately describe photon migration in layered media; however, storing and querying the resulting dataset may be computationally prohibitive when detailed path data are needed for each photon trajectory. A heuristic approach that significantly reduces the stored information to the average path length traveled by the photons detected in each layer is proposed. Its accuracy is evaluated by comparing it with the exact time point spread function (*TPSF*) for a bilayered medium. This method, almost exact for small variations in absorption, is potentially useful to provide a small dataset for lookup tables to be used in inverse problems.

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The description of a bilayer geometry is of considerable interest in the field of tissue optics. In fact, it is representative, e.g., of the layer of fat overlying the muscle tissue [1,2], of the extracerebral tissue over the brain [3–5], or of the chest over the lungs [6,7]. Several methods to model photon propagation in turbid stratified media are available, among which analytical solutions of the diffusion equation (DE), Monte Carlo (MC) simulations, or a hybrid approach between the two [8–17]. Nevertheless, for high absorption values, the DE may not be accurate at early times and/or short source-detector distances, while MC methods, although rigorous, are lengthy and require considerable computational resources. A way to reduce the processing time of forward or inverse problems involving MC simulations is to store them in a lookup table for suitable scattering and absorption values [18–22]. However, if the medium is heterogeneous, the stored information becomes enormous, due to all the possible combinations of optical properties for the various layers that have to be taken into account. Another approach is to create a lookup table that encompasses only scattering values and then exploiting the microscopic Beer–Lambert–Bouguer law to introduce the effects of absorption. However, this method still necessitates storing the partial path lengths (PP) traveled in each layer by the potentially millions of detected photons, again leading to a substantial increase in the amount of stored data.

The aim of this work is to prove the feasibility of reducing the quantity of stored information necessary to calculate the absorption properties of the heterogeneous medium. In particular, we propose a heuristic model with enough accuracy and, at the same time, low computational load, which relies on the knowledge of the mean values of the PP traveled inside each layer of the medium, instead of the PP of every photon.

In MC methods, an already common practice to account for the absorption of the medium consists in weighting each trajectory of a simulation performed in a non-absorbing medium (*white* simulation [19,23]) with an exponential factor that considers the path lengths traveled in each subvolume of the medium. In the time-domain approach, the weights of each trajectory are separated into time bins and then summed together within each bin in order to obtain the time point spread function (*TPSF*).

It would be beneficial to find a method that allows to straightforwardly scale the white *TPSF* ($TPSF_0$) instead of relying on the information of all the simulated photon trajectories. This is trivial in the case of homogeneous media, while for heterogeneous ones, the PP of each photon are required.

If we consider a bilayered medium, the scaled *TPSF* can be rigorously obtained as follows [24]:

$$TPSF(\mu_{a0}, \mu_{a1}, t) = TPSF_0 \cdot \int_0^{vt} f_0(l_0, l_1, t) \exp(-\mu_{a0} l_0) \cdot \cdot \exp(-\mu_{a1} l_1)\, dl_0, \tag{1}$$

with the constraint $l_1 = vt - l_0$. In Eq. (1), $TPSF_0$ is the *TPSF* relative to the non-absorbing case, i.e., for $\mu_{a0} = \mu_{a1} = 0$, v is the speed of light in the medium. In particular, in order to not overload the notation, Eq. (1) is relative to the case of equal refractive indices in the two layers. However, the implementation with different refractive indices is straightforward.

For the non-absorbing medium, the function $f_0(l_0, l_1, t)$ is the probability distribution of the PP l_0 and l_1 spent in the first and second layer, respectively, by a photon received at time t. We stress that this function also depends on the source-detector distance, the thicknesses of the layers, and their scattering properties and refractive indices. For the sake of brevity, this information is omitted in the notation, as well as the dependence of l_0 and l_1 from the time t considered at the detection site.

Equation (1) is exact; however, since $f_0(l_0, l_1, t)$ is unknown, the integral cannot be calculated. One option may be to reconstruct $f_0(l_0, l_1, t)$ through MC simulations, once fixed the geometrical and optical properties of the non-absorbing medium. Therefore, if we consider a lookup table approach, we must also store for each $TPSF_0$ the distribution function $f_0(l_0, l_1, t)$, reconstructed by means of the PP of the received photons, with sufficient sampling to guarantee the convergence of the integral.

In this work, we show that Eq. (1) can be approximated, with enough accuracy, by the heuristic expression:

$$TPSF(\mu_{a0}, \mu_{a1}, t) \approx TPSF_0 \cdot \exp\left(-\mu_{a0}\bar{l}_0\right) \cdot \exp\left(-\mu_{a1}\bar{l}_1\right), \quad (2)$$

where the mean paths $\bar{l}_0$ and $\bar{l}_1$, traveled by photons received at time t in the first and second layer, are calculated for absorption coefficients $\frac{\mu_{a0}}{2}$ and $\frac{\mu_{a1}}{2}$, respectively, which are the absorption values halfway between those of the initial $TPSF_0$ and of the final scaled $TPSF$:

$$\bar{l}_0(t) = \int_0^{vt} dl_0\, l_0 f\left(l_0, l_1, t; \frac{\mu_{a0}}{2}, \frac{\mu_{a1}}{2}\right), \quad (3)$$

$$\bar{l}_1(t) = \int_0^{vt} dl_1\, l_1 f\left(l_0, l_1, t; \frac{\mu_{a0}}{2}, \frac{\mu_{a1}}{2}\right), \quad (4)$$

with the constraint $l_1 = vt - l_0$ for Eq. (3) and $l_0 = vt - l_1$ for Eq. (4).

In the following, we will justify the reasonability of the approximation reported in Eq. (2). First, let us assume infinitesimal values for the absorption of the two layers, i.e., $\mu_{a0} = \delta\mu_{a0}$ and $\mu_{a1} = \delta\mu_{a1}$. In this case, the integral in Eq. (1) can be explicitly calculated:

$$\begin{aligned} TPSF &= TPSF_0 \int_0^{vt} dl_0 f_0(l_0, l_1, t) \cdot \exp\{-\delta\mu_{a0} l_0 - \delta\mu_{a1} l_1\} \approx \\ &\approx TPSF_0 \int_0^{vt} dl_0 f_0(l_0, l_1, t) \cdot \{1 - \delta\mu_{a0} l_0 - \delta\mu_{a1} l_1\} = \\ &= TPSF_0 \cdot \{1 - \delta\mu_{a0}\langle l_0\rangle_0 - \delta\mu_{a1}\langle l_1\rangle_0\}, \end{aligned} \quad (5)$$

where $\langle l_0\rangle_0$ and $\langle l_1\rangle_0$ represent the average photon path lengths in the two layers:

$$\langle l_0\rangle_0 = \int_0^{vt} dl_0\, l_0 f_0(l_0, l_1, t)\,, \quad (6)$$

$$\langle l_1\rangle_0 = \int_0^{vt} dl_1\, l_1 f_0(l_0, l_1, t)\,. \quad (7)$$

Now, we can rewrite Eq. (5) back into the exponential form:

$$TPSF = TPSF_0 \cdot \exp\{-\delta\mu_{a0}\langle l_0\rangle_0 - \delta\mu_{a1}\langle l_1\rangle_0\}\,. \quad (8)$$

In other words, the approximation in Eq. (2) is effective provided that $\delta\mu_{a0}\langle l_0\rangle_0 + \delta\mu_{a1}\langle l_1\rangle_0 \ll 1$. The quantities $\delta\mu_{a0}$ and $\delta\mu_{a1}$ are always positive.

Let us now consider finite values for the absorption coefficients μ_{a0} and μ_{a1}. The idea is to break them down into N small increments $\Delta\mu_{a0}$ and $\Delta\mu_{a1}$:

$$\Delta\mu_{a0} = \frac{\mu_{a0}}{N}, \quad \Delta\mu_{a1} = \frac{\mu_{a1}}{N}, \quad (9)$$

in such a way that we can consider steps of increasing absorption as follows:

$$\mu_{a0i} = i\Delta\mu_{a0} = \frac{i}{N}\mu_{a0}, \quad \mu_{a1i} = i\Delta\mu_{a1} = \frac{i}{N}\mu_{a1}, \quad (10)$$

for $i = 1, \ldots, N$, to get the absorption values μ_{a0} and μ_{a1}.

This implies that we can introduce the effect of the overall absorption on $TPSF$ by considering successive steps i, applying each time Eq. (1). It is crucial that we choose N sufficiently large, so that for each step, the absorption variation is small enough for the scaling to be efficient. An iterative approach is required because at each step, the path distribution function $f(l_0, l_1, t)$ needs to be updated with the new current values of the absorption in the two layers. Following this principle, with a few more steps, we get the following:

$$\begin{aligned} TPSF(\mu_{a0}, \mu_{a1}, t) &= TPSF_0 \cdot \\ &\cdot \prod_{i=1}^{N} \exp\{-\Delta\mu_{a0}\langle l_0\rangle_i - \Delta\mu_{a1}\langle l_1\rangle_i\}. \end{aligned} \quad (11)$$

The notation $\langle l_0\rangle_i$ is a generalization of Eq. (6) and indicates the mean path in the first layer when the absorption in the first and second layer are $\mu_{a0,i-1}$ and $\mu_{a1,i-1}$, respectively. Similarly, for $\langle l_1\rangle_i$. In other words, it results in the following:

$$\langle l_0\rangle_i = \int_{\substack{0\le l_0\le vt \\ l_1 = vt - l_0}} dl_0\, l_0 f_{i-1}(l_0, l_1, t)\,, \quad (12)$$

$$\langle l_1\rangle_i = \int_{\substack{0\le l_1\le vt \\ l_0 = vt - l_1}} dl_1\, l_1 f_{i-1}(l_0, l_1, t)\,, \quad (13)$$

where we set the following:

$$f_i(l_0, l_1, t) = f(l_0, l_1, t; \mu_{a0i}, \mu_{a1i})\,. \quad (14)$$

Thus, Eq. (11) can be recast as follows:

$$\begin{aligned} TPSF &= TPSF_0 \exp\left\{\sum_{i=1}^{N}(-\Delta\mu_{a0}\langle l_0\rangle_i - \Delta\mu_{a1}\langle l_1\rangle_i)\right\} = \\ &= TPSF_0 \exp\left\{-\Delta\mu_{a0} N \frac{\sum_{i=1}^{N}\langle l_0\rangle_i}{N} - \Delta\mu_{a1} N \frac{\sum_{i=1}^{N}\langle l_1\rangle_i}{N}\right\} = \\ &= TPSF_0 \exp\left\{-\mu_{a0}\frac{\sum_{i=1}^{N}\langle l_0\rangle_i}{N} - \mu_{a1}\frac{\sum_{i=1}^{N}\langle l_1\rangle_i}{N}\right\}. \end{aligned} \quad (15)$$

It can be seen that Eq. (2) is justified provided that the summations on the average paths in Eq. (15) can be replaced with the mean paths $\bar{l}_0$ and $\bar{l}_1$ of Eqs. (3) and (4), respectively. Then, we have to show the following:

$$\frac{\sum_{i=1}^{N}\langle l_0\rangle_i}{N} \approx \bar{l}_0\,, \quad (16)$$

$$\frac{\sum_{i=1}^{N}\langle l_1\rangle_i}{N} \approx \bar{l}_1\,. \quad (17)$$

If we use now Eq. (12) to develop the summation on the average paths in Eq. (16), we obtain the following:

$$\begin{aligned} \frac{1}{N}\sum_{i=1}^{N}\langle l_0\rangle_i &= \frac{1}{N}\sum_{i=1}^{N}\int_{\substack{0\le l_0\le vt \\ l_1 = vt - l_0}} dl_0\, l_0 f_{i-1}(l_0, l_1, t) = \\ &= \frac{1}{\mu_{a0}}\int_{\substack{0\le l_0\le vt \\ l_1 = vt - l_0}} dl_0\, l_0 \sum_{i=1}^{N}\frac{\mu_{a0}}{N} f_{i-1}(l_0, l_1, t) = \\ &= \frac{1}{\mu_{a0}}\int_{\substack{0\le l_0\le vt \\ l_1 = vt - l_0}} dl_0\, l_0 \sum_{i=1}^{N}\Delta\mu_{a0} f_{i-1}(l_0, l_1, t). \end{aligned} \quad (18)$$

When $N \to \infty$ (and $\Delta\mu_{a0} \to 0$), we can write the following:

$$\frac{1}{N}\sum_{i=1}^{N}\langle l_0\rangle_i = \int_{\substack{0\le l_0\le vt\\ l_1=vt-l_0}} dl_0\, l_0\, \frac{1}{\mu_{a0}}\int_0^{\mu_{a0}} d\mu'_{a0} f(l_0, l_1, t; \mu'_{a0}, \mu'_{a1}), \quad (19)$$

where $\mu'_{a1} = \mu'_{a0}\frac{\mu_{a1}}{\mu_{a0}}$. Then, by substituting Eqs. (3) and (19) in Eq. (16), the latter results are equivalent to the following relation:

$$\frac{1}{\mu_{a0}}\int_0^{\mu_{a0}} d\mu'_{a0} f(l_0, l_1, \mu'_{a0}, \mu'_{a1}, t) \approx f\left(l_0, l_1, t; \frac{\mu_{a0}}{2}, \frac{\mu_{a1}}{2}\right). \quad (20)$$

Following a similar derivation, one can demonstrate that Eq. (17) is equivalent to the following:

$$\frac{1}{\mu_{a1}}\int_0^{\mu_{a1}} d\mu'_{a1} f(l_0, l_1, \mu'_{a0}, \mu'_{a1}, t) \approx f\left(l_0, l_1, t; \frac{\mu_{a0}}{2}, \frac{\mu_{a1}}{2}\right). \quad (21)$$

Finally, it can be noted that the analytical form of Eq. (2) recalls that of the Rytov and Born approximation, which also uses the information on the mean path length spent by the received light in an absorbing volume [24]. Unlike the Born and Rytov approximation, we used the mean values of the path lengths at the midpoint between initial and final absorption values. This mitigates the effects of the dependence of mean path lengths on absorption.

The heuristic expression reported in Eq. (2) is compared with the exact *TPSF* obtained from MC simulations. Let us consider a two-layer semi-infinite medium composed of a superficial layer and a bulk. As for the MC simulations, we exploited a MATLAB tool provided by Fang *et al.* [25]. We calculated the approximated *TPSF* in Eq. (2) starting from a white MC simulation and estimating the mean PP $\bar{l}_0$ and $\bar{l}_1$ for different values of the absorption coefficient of the layers.

The MC simulations were performed for isotropic scattering considering several two-layer media, with a first layer thickness $s_1 \in [2, 8]$ mm and source-detector distances of 10 mm and 20 mm. Moreover, various scattering coefficients were considered, either equal and different within the two layers. For brevity, we have reported only few representative cases in Fig. 1.

It can be clearly observed from Fig. 1 that the error of the heuristic model, estimated by the ratio between the *TPSF* calculated with the heuristic model and the exact MC simulation, is negligible for early arrival times (lower than 500 ps), remaining always lower than 10% for late arrival times, except for the last case considered (fourth column), where it reaches 50%.

For a better understanding of the errors in the heuristic model shown in Fig. 1, in Fig. 2 the mean PP $\langle l_0\rangle$ and $\langle l_1\rangle$ are plotted as a function of the absorption coefficients, for different photon arrival times. We have previously shown, in fact, that the heuristic model reported in Eq. (2) can be considered exact if Eqs. (20) and (21) are verified. This is true if the dependence of the distribution $f(l_0, l_1, \mu_{a0}, \mu_{a1}, t)$ on μ_{a0} and μ_{a1} is linear. If this is the case, also $\langle l_0\rangle$ and $\langle l_1\rangle$ traveled by photons in each layer are linearly dependent from μ_{a0} and μ_{a1}, respectively.

From Fig. 2, we can first see that $\langle l_0\rangle$ and $\langle l_1\rangle$ are longer for small absorption coefficients and became increasingly shorter as the absorption coefficients increase, as expected. Moreover, for the first arrival times, this decreasing trend is almost linear, ensuring good accuracy of the heuristic model, as shown in Fig. 1. When considering the late arrival times, however, an increasingly evident nonlinear dependence of $\langle l_0\rangle$ and $\langle l_1\rangle$ on the absorption coefficients is observed, justifying the increased inaccuracy of the heuristic model for the late arrival times.

To conclude, we have presented a heuristic model for scaling a time-resolved white MC simulation considering the absorption effect in a heterogeneous medium, with the advantage that it is not necessary to record all partial paths traveled by photons, but only their average values. This reduces both the size of the stored dataset and its processing time. If we consider, as

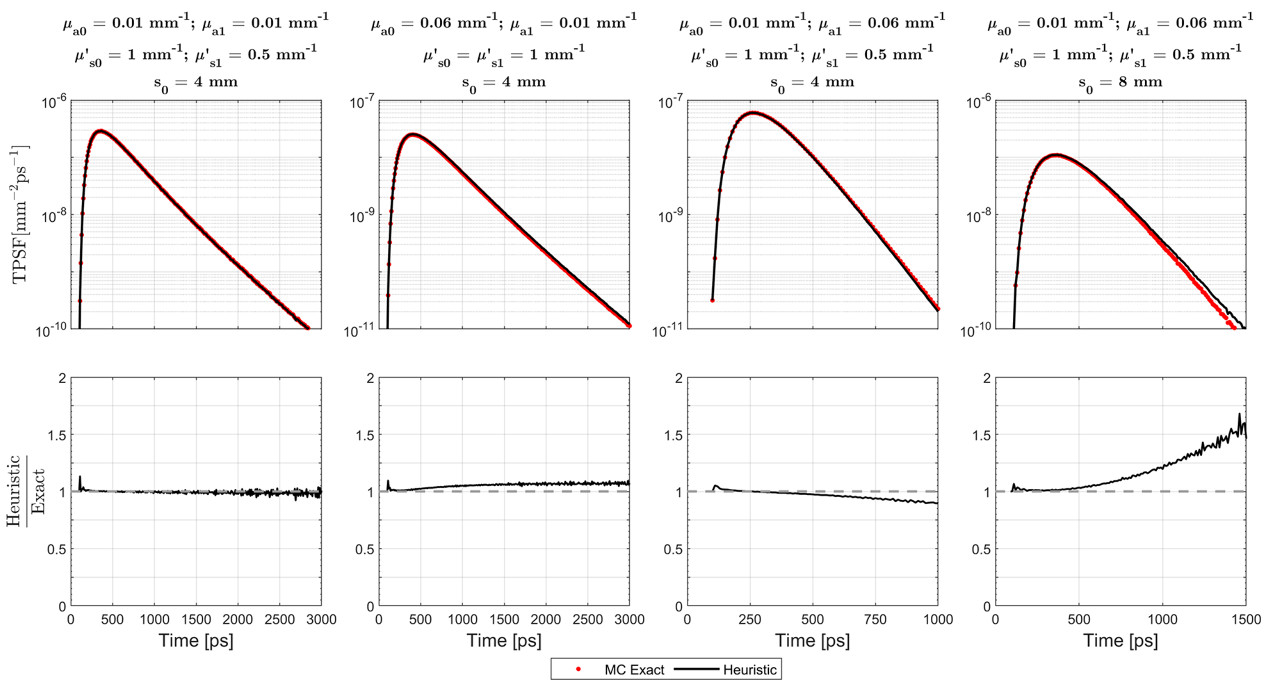

Fig. 1. First row: comparison between *TPSF* obtained in a two-layer medium in reflectance geometry by the heuristic approach (black line) and by a MC simulation (red line). Second row: ratio between the heuristic and exact *TPSF*. Common parameters: thickness of the second layer $s_1 = 40$ mm, refractive indices $n_{ext} = 1$ and $n_0 = n_1 = 1.4$, isotropic scattering, and source-detector distance $\rho = 20$ mm. The optical properties of both layers and the thickness of the first layer are indicated in the header of each column.

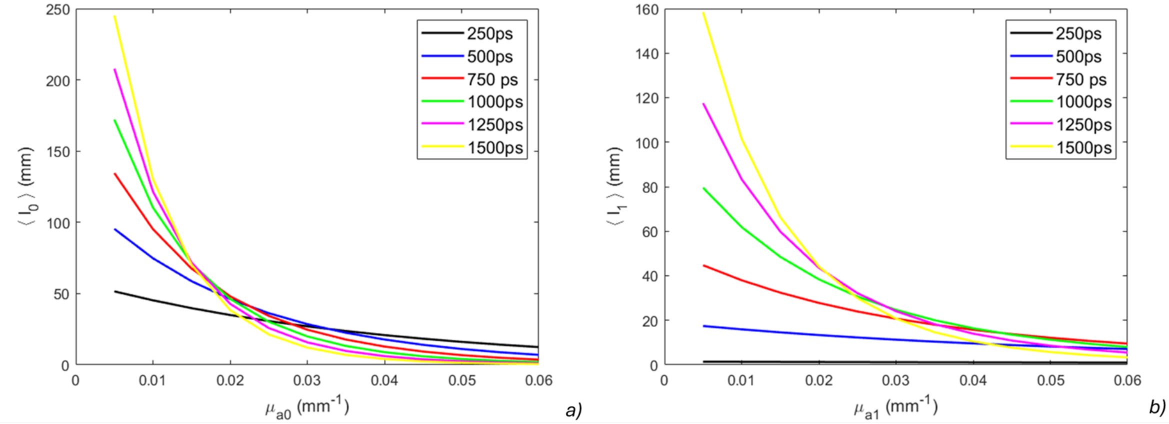

Fig. 2. Mean PP $\langle l_0 \rangle$ and $\langle l_1 \rangle$ as a function of the absorption coefficient, for different photon arrival times, calculated for a two-layer medium by a MC tool. Common parameters: source-detector distance $\rho = 20$ mm, layer thicknesses $s_0 = 8$ mm and $s_1 = 40$ mm, isotropic scattering, reduced scattering coefficients $\mu'_{s0} = 1$ mm^{-1} and $\mu'_{s1} = 0.5$ mm^{-1}, and refractive indices $n_0 = n_1 = 1.4$. Panel (a): $\mu_{a1} = 0.06$ mm^{-1}, Panel (b): $\mu_{a0} = 0.01$ mm^{-1}. Subscript 0 and 1 refer to first and second layer, respectively.

an example, a bilayer medium and 10^7 white detected photons, the size of the MC dataset scales as $2 \cdot 10^7$, while for a 200 time bin $TPSF_0$ and a 10×10 mean path length lookup table, the size of the heuristic model dataset scales as $4 \cdot 10^4$. Correspondingly, the *TPSF* simulation time reduces by about 70 times, when a workstation equipped with an Intel® Xeon® Processor E5-2670 v3 @2.30 GHz and 192 GB RAM @2133 MHz is exploited.

We note that this approach can also be used for scaling analytical models. The accuracy of this approach was tested in the case of a two-layer medium exploiting a MC tool with encouraging results, especially for early arrival times.

On the comprehension viewpoint, we can assess that the heuristic model presented can also be considered as a further step forward in the description of the propagation of light in diffusive heterogeneous media. From an application point of view, when dealing with inversion problems on heterogeneous media, the presented heuristic model can be profitably utilized, considering its reduced storing requirements and fast computational times, which are crucial features for the development of inversion algorithms.

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Data availability. Data underlying the results presented in this paper are not publicly available at this time but may be obtained from the authors upon reasonable request.

REFERENCES

1. I. Pirovano, S. Porcelli, R. Re, *et al.*, Biomed. Opt. Express **12**, 571 (2021).
2. Y. Matsuda, M. Nakabayashi, T. Suzuki, *et al.*, Front. Bioeng. Biotechnol. **9**, 800051 (2022).
3. L. Contini, C. Amendola, D. Contini, *et al.*, Neurophotonics **11**, 035001 (2024).
4. T.-C. Kao and K.-B. Sung, J. Biomed. Opt. **27**, 083021 (2022).
5. M. M. Wu, K. Perdue, S.-T. Chan, *et al.*, Biomed. Opt. Express **13**, 1131 (2022).
6. A. Pifferi, M. Miniati, A. Farina, *et al.*, Sci. Rep. **14**, 6343 (2024).
7. J. Guo, S. Meng, H. Su, *et al.*, Biomed. Opt. Express **13**, 6389 (2022).
8. F. Martelli, A. Sassaroli, S. Del-Bianco, *et al.*, Phys. Med. Biol. **52**, 2827 (2007).
9. X. Wang, Optik **180**, 144 (2019).
10. L. Gagnon, M. Desjardins, J. Jehanne-Lacasse, *et al.*, Opt. Express **16**, 15514 (2008).
11. M. Helton, S. Zerafa, K. Vishwanath, *et al.*, Sci. Rep. **12**, 18979 (2022).
12. M. Sharma, R. Hennessy, M. K. Markey, *et al.*, Biomed. Opt. Express **5**, 40 (2014).
13. A. Liemert and A. Kienle, J. Biomed. Opt. **15**, 025002 (2010).
14. J. Kangasniemi, M. Mozumder, A. Pulkkinen, *et al.*, Biomed. Opt. Express **15**, 4925 (2024).
15. G. Alexandrakis, T. J. Farrell, and M. S. Patterson, Appl. Opt. **39**, 2235 (2000).
16. H. Fujii, S. Okawa, Y. Yamada, *et al.*, J. Quant. Spectrosc. Radiat. Transfer **147**, 145 (2014).
17. M. Kervella, T. Tarvainen, A. Humeau, *et al.*, *Proceedings of the 5th WSEAS Int. Conf. on System Science and Simulation in Engineering* (2006).
18. A. Pifferi, P. Taroni, G. Valentini, *et al.*, Appl. Opt. **37**, 2774 (1998).
19. E. Alerstam, S. Andersson-Engels, and T. Svensson, J. Biomed. Opt. **13**, 041304 (2008).
20. R. J. Hennessy, S. L. Lim, M. K. Markey, *et al.*, J. Biomed. Opt. **18**, 037003 (2013).
21. X. Zhong, X. Wen, and D. Zhu, Opt. Express **22**, 1852 (2014).
22. P. Naglič, M. Bregar, F. Pernuš, *et al.*, Proc. SPIE **9333**, 71 (2015).
23. C. Amendola, G. Maffeis, A. Farina, *et al.*, Opt. Express **32**, 125 (2024).
24. A. Sassaroli, F. Martelli, and S. Fantini, J. Opt. Soc. Am. A **23**, 2105 (2006).
25. Y. Zhang and Q. Fang, J. Biomed. Opt. **27**, 083014 (2022).