Adding scattering for photon migration: exact identities and experimental validation

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Adding scattering for photon migration: exact identities and experimental validation

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Abstract: Exact identities for radiative transfer are derived in scattering and absorbing media that relate emitted, received, and absorbed power (in the full domain or in arbitrary sub-volumes) to two trajectory statistics: the mean optical pathlength $\langle \ell \rangle$ traveled by photons and the mean number of scattering events $\langle k \rangle$. For the received signal, the logarithmic derivatives with respect to absorption and scattering take particularly simple forms. In the continuous-wave case, $\partial \ln (P_\mathrm{R}) / \partial \mu_\mathrm{a} = -\langle \ell \rangle_\mathrm{R}$ and $\partial \ln (P_\mathrm{R}) / \partial \mu_s = \langle k \rangle_\mathrm{R} / \mu_s - \langle \ell \rangle_\mathrm{R}$, with analogous relations for time-resolved measurements. The second identity implies a counter-intuitive and yet highly consequential fact: the difference $\langle k \rangle_\mathrm{R} / \mu_s - \langle \ell \rangle_\mathrm{R}$ is generally nonzero, which is required to ensure that the detected signal is sensitive to scattering variations. Motivated by this observation, we formalize an "adding scattering" protocol, analogous to established adding-absorption approaches, to estimate scattering sensitivity via finite-difference changes in μ_s in both Monte Carlo simulations and experiments. The predicted relations are validated via independent Monte Carlo implementations and with measurements in calibrated liquid phantoms. Finally, the role of these identities as exact benchmarks for forward solvers in photon migration studies is discussed.

1. Introduction

The radiative transfer equation (RTE) [1–4] is an exact theoretical framework widely recognized as a benchmark for generating precise photon transport solutions. These solutions are applied across numerous fields, including tissue optics [5–8]. In practical applications, having exact solutions and relationships derived from the RTE is indeed crucial.

Analytical solutions of the RTE are currently limited to specific geometries and types of illumination [9–12], and their computation requires substantial computational effort. Relevant reference solutions for the RTE have also been derived under the special condition of non-absorbing media uniformly illuminated by Lambertian light [13–17]. This scenario involves incident uniform isotropic radiance across the entire external surface of the medium, a unique condition in radiative transfer that allows detailed description of light propagation for any radiometric quantity [17]. These solutions serve as fundamental benchmarks for validating forward solvers, such as Monte Carlo (MC) codes [18].

In this study, we leverage the intrinsic physical meanings of the absorption coefficient, scattering coefficient, and scattering function — fundamental components of the radiative transfer equation — to derive two sets of exact formal relations that hold, without approximation, for photon transport described within the RTE framework, irrespective of geometry, source configuration,

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or detector arrangement. As customary in radiative transfer theory, the treatment refers to classical, incoherent light propagation, for which absorption and scattering can be characterized by macroscopic coefficients.

These relationships establish connections between the power emitted, absorbed, and received within any scattering and absorbing medium, as well as within any of its sub-volumes. They relate these quantities to the average path length traveled by emitted photons, the average number of scattering events underwent by those photons, and the average photon fluence rate. As a result, they form a set of interconnected relationships, offering multiple ways to understand propagation through simple and elementary mathematics. This avoids the need for complex Radiative Transfer Equation (RTE) solutions, which often lack intuitive understanding.

While the basic structure behind these relations is connected to perturbation and scaling ideas used in Monte Carlo photon transport, the present work unifies a set of exact identities for received and absorbed power (in both homogeneous and heterogeneous media), discussing their physical consequences. To the best of our knowledge, this set of relationships in the form presented here has never been recognized in previous literature. A direct consequence of these identities is the formulation of an "adding scattering" protocol, as a counterpart to the known "adding absorption" method, that provides a practical route to estimate the scattering sensitivity of a detected signal in simulations and experiments. A central outcome is that, for received power, the quantity $\langle k\rangle_{\mathrm{R}}/\mu_{\mathrm{s}} - \langle \ell\rangle_{\mathrm{R}}$ is in general not zero. This shows that this commonly held heuristic assumption in the diffusive regime is not exact for detected photons, and it further demonstrates that their exact equivalence would actually imply vanishing sensitivity to μ_{s}. The paper is organized into two parts: the derivations (Section 2) and representative applications (Section 3), including conceptual examples (Subsections 3.1 and 3.2), Monte Carlo validation (Subsection 3.3), and an experimental demonstration of "adding scattering" (Subsection 3.4).

2. Theory

This work employs the concept of photon trajectories, calculated using the general statistical principles governing fundamental phenomena in radiative transfer theory, such as absorption and scattering interactions. This approach effectively simulates the exact statistical physics of energy transport within the medium under consideration. The derived relations are categorized into two groups: 1) Those pertaining to received power and its logarithmic derivatives (Subsection 2.1 and 2.3); 2) Those related to absorbed power and its logarithmic derivatives (Subsections 2.2 and 2.5). In Subsection 2.7, we introduce the method of "adding absorption" and a novel approach termed "adding scattering". These methods establish connections between the variations in received signals due to changes in absorption and scattering within the medium. Finally, the obtained relations are combined to consider the total power and its logarithmic derivatives (Subsections 2.3 and 2.6).

Notation and conventions. To keep the notation compact and consistent across the presentation of the results, we use a number of recurring subscripts and superscripts. Since the same base symbol may appear in several variants (e.g. received vs. absorbed, total vs. restricted to a sub-volume, or conditioned on a fixed scattering order), we summarize our conventions here for ease of reference. We use the placeholder symbol $\square$ to denote a generic quantity to which subscripts/superscripts may be attached. Subscripts indicate the power type: $\square_{\mathrm{E}}$ (emitted), $\square_{\mathrm{R}}$ (received), $\square_{\mathrm{A}}$ (absorbed). Index i denotes a sub-volume $V_i \subseteq V$ in heterogeneous media (e.g., $\square_i$). Subscript k denotes conditioning on a fixed number of scattering events (e.g., $\square_k$ or $\square_{\mathrm{R},k}$). Superscript $\square^{\mathrm{T}}$ denotes "total" (i.e. integrated over the full domain or over all escaping directions, as appropriate). Superscripts $\square^*$ and $\square^\dagger$ denote quantities restricted to V_i and to its complement within $\overline{V}$, respectively, when a decomposition $\overline{V} = V_i \cup V^\dagger$ is used. A tilde (e.g. $\tilde{\square}$) denotes a single-trajectory contribution. An overline (e.g. $\overline{\square}$) denotes a quantity related to a volume $\overline{V}$.

2.1. Homogeneous medium: the received power

In this section, we derive the basic relationships describing the sensitivity of the received light power on absorption and scattering coefficients, for a general homogeneous medium. The obtained relationships are of general interest due to their independence from the position of the sources and detectors, as well as from the medium geometry.

The theory presented in this section, for the simple homogeneous case, will also serve as the basis to tackle the more complex heterogeneous case, presented in Section 2.4.

2.1.1. Basic relationships

Let V be a homogeneous domain characterized by a refractive index, absorption and scattering properties, including discrete and/or continuous light sources and detectors. Surface emitting light sources or surface detectors may be distributed anywhere on the surface of V. Volume emitting light sources or volume detectors may be distributed anywhere inside V. This section presents a derivation of the functional dependence of the received power from the optical properties of the medium and light sources.

Let $\mathrm{d}\tilde{P}_{\mathrm{R}_k}$ be the fraction of the power $\mathrm{d}P_{\mathrm{E}}$ (see Fig. 1) — emitted by a surface light source element $\mathrm{d}\Sigma_{\mathrm{S}}$, within the solid angle $\mathrm{d}\hat{\mathbf{s}}_0$ — that is received by the surface element $\mathrm{d}\Sigma_{\mathrm{R}}$ of the receiver, after k scattering events. As it is well known, $\mathrm{d}\tilde{P}_{\mathrm{R}_k}$ can be expressed as [8]:

$$\begin{aligned}\mathrm{d}\tilde{P}_{\mathrm{R}_k} =&\mathrm{d}P_{\mathrm{E}}\, \mathrm{e}^{-(\mu_{\mathrm{a}}+\mu_{\mathrm{s}})\ell_1}\mu_{\mathrm{s}}\mathrm{d}\ell_1 p(\hat{\mathbf{s}}_1,\hat{\mathbf{s}}_0)\mathrm{d}\hat{\mathbf{s}}_1 \times \mathrm{e}^{-(\mu_{\mathrm{a}}+\mu_{\mathrm{s}})\ell_2}\mu_{\mathrm{s}}\mathrm{d}\ell_2 p(\hat{\mathbf{s}}_2,\hat{\mathbf{s}}_1)\mathrm{d}\hat{\mathbf{s}}_2 \times \cdots \\ &\times \mathrm{e}^{-(\mu_{\mathrm{a}}+\mu_{\mathrm{s}})\ell_{k-1}}\mu_{\mathrm{s}}\mathrm{d}\ell_{k-1} p(\hat{\mathbf{s}}_{k-1},\hat{\mathbf{s}}_{k-2})\mathrm{d}\hat{\mathbf{s}}_{k-1} \times \mathrm{e}^{-(\mu_{\mathrm{a}}+\mu_{\mathrm{s}})\ell_k}\mu_{\mathrm{s}}\mathrm{d}\ell_k p(\hat{\mathbf{s}}_k,\hat{\mathbf{s}}_{k-1})\mathrm{d}\hat{\mathbf{s}}_k \times \mathrm{e}^{-(\mu_{\mathrm{a}}+\mu_{\mathrm{s}})\ell_{k+1}},\end{aligned} \tag{1}$$

where $p(\cdot,\cdot)$ is the scattering function of the medium, μ_{s} the scattering coefficient, μ_{a} the absorption coefficient and $\mathrm{d}\hat{\mathbf{s}}_k$ the solid angle element which subtends the receiver element $\mathrm{d}\Sigma_{\mathrm{R}}$.

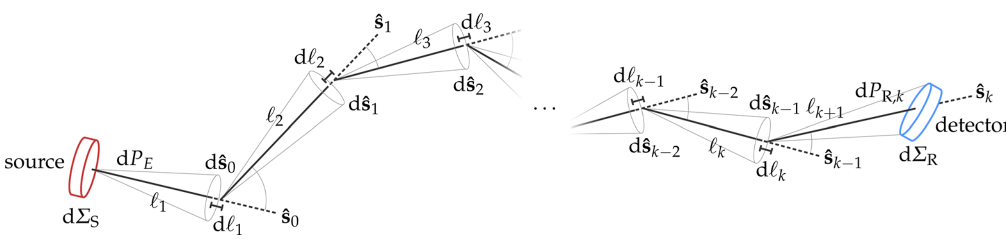

Fig. 1. Example of trajectory, with k scattering events, traveled by the emitted power $\mathrm{d}P_{\mathrm{E}}$ to reach the receiver element $\mathrm{d}\Sigma_{\mathrm{R}}$. Although, for simplicity, the figure shows a 2D representation, we refer in general to a 3D propagation.

Equation (1) can intuitively be understood by noting that $\exp[-(\mu_{\mathrm{a}} + \mu_{\mathrm{s}})\ell_i]$ represents the fraction of remaining power due to absorption and scattering events, at the end of a path of length ℓ_i. The term $\mu_{\mathrm{s}}\mathrm{d}\ell_i$ represents the probability to be scattered along a path of length $\mathrm{d}\ell_i$; and $p(\hat{\mathbf{s}}_i,\hat{\mathbf{s}}_{i-1})\mathrm{d}\hat{\mathbf{s}}_i$ the probability to be scattered from direction $\hat{\mathbf{s}}_{i-1}$ to direction $\hat{\mathbf{s}}_i$, within the solid angle $\mathrm{d}\hat{\mathbf{s}}_i$. More formally, Eq. (1) is basically a general summand of the Neumann series solution in integral form of the RTE [19]. The Neumann series solves the RTE by representing the total intensity as a sum of scattering orders, expanding the solution into an iterative series where each term represents photons scattered $0, 1, 2, \ldots, k$ times.

Then, Eq. (1) can be synthetically re-written as:

$$\mathrm{d}\tilde{P}_{\mathrm{R}_k} = \mathrm{d}P_{\mathrm{E}}\mu_{\mathrm{s}}^k \mathrm{e}^{-(\mu_{\mathrm{a}}+\mu_{\mathrm{s}})\ell} \prod_{i=1}^{k} \mathrm{d}\ell_i p(\hat{\mathbf{s}}_i,\hat{\mathbf{s}}_{i-1})\mathrm{d}\hat{\mathbf{s}}_i, \tag{2}$$

where $\ell = \sum_{i=1}^{k+1} \ell_i$.

The fraction of power $\mathrm{d}P_\mathrm{E}$ emitted in the solid angle $\mathrm{d}\hat{\mathbf{s}}_0$, for a *surface* emitting source, can be expressed as $\mathrm{d}P_\mathrm{E} = P_\mathrm{E}(\boldsymbol{r}_s, \hat{\mathbf{s}}_0)\mathrm{d}\Sigma_S \mathrm{d}\hat{\mathbf{s}}_0$, with $P_\mathrm{E}(\boldsymbol{r}_s, \hat{\mathbf{s}}_0)$ representing the power emitted per unit area at $\boldsymbol{r}_s$ and unit solid angle along $\hat{\mathbf{s}}_0$.

Equation (2) can be also written for a *volume* emitting source, with volume element $\mathrm{d}V_S$, and $\mathrm{d}P_\mathrm{E} = P_\mathrm{E}(\boldsymbol{r}_s, \hat{\mathbf{s}}_0)\mathrm{d}V_S \mathrm{d}\hat{\mathbf{s}}_0$, with the function $P_\mathrm{E}(\boldsymbol{r}_s, \hat{\mathbf{s}}_0)$ representing in this case the power emitted per unit volume at $\boldsymbol{r}_s$ and unit solid angle along $\hat{\mathbf{s}}_0$.

The total power $\mathrm{d}P_{\mathrm{R}_k}$ received from trajectories with k scattering events and total length between ℓ and $\ell + \mathrm{d}\ell$ is obtained by summing the contributions $\mathrm{d}\tilde{P}_{\mathrm{R}_k}$ in the space of possible trajectories. In practice, this is achieved by integrating Eq. (2) on: 1) all possible trajectories with k scattering events and length between ℓ and $\ell + \mathrm{d}\ell$, connecting a source element with a receiver element; 2) all source distributions and; 3) the whole extent and field of view of the receiver. Thus, $\mathrm{d}P_{\mathrm{R}_k}$ can be expressed as:

$$\mathrm{d}P_{\mathrm{R}_k}(\ell) = P_\mathrm{E} C_{\mathrm{R}_k}(\ell)\mu_\mathrm{s}^k \mathrm{e}^{-(\mu_\mathrm{a}+\mu_\mathrm{s})\ell}\mathrm{d}\ell, \tag{3}$$

where P_E is the total power emitted by the sources and $C_{\mathrm{R}_k}(\ell)$ is a coefficient that depends on ℓ and many other factors (e.g., source and receiver geometries, medium geometry, scattering function, internal and external refractive indexes). However, it is important to note that $C_{\mathrm{R}_k}(\ell)$ is *independent* of μ_a and μ_s.

Although the analytical calculation of $C_{\mathrm{R}_k}(\ell)$ is typically unfeasible in situations of practical interest, Eq. (3) remains important because it explicitly gives the exact dependence of $\mathrm{d}P_{\mathrm{R}_k}(\ell)$ on the scattering and absorption coefficients of the medium, through the term $\mu_\mathrm{s}^k \mathrm{e}^{-(\mu_\mathrm{a}+\mu_\mathrm{s})\ell}$. This is the key point for obtaining the relationships presented in this contribution. In the context of RTE theory, Eq. (3) represents an exact expression that is exempt of approximations.

Equations (2) and (3) have been derived for a medium with *uniform* refractive index. In a medium with *non-uniform* refractive index, we must also take into account the fact that the trajectories are also affected by reflection and refraction at the interfaces of different sub-domains. However, Eqs. (2) and (3) remain valid even in this case, provided that the term ℓ is interpreted appropriately (see Subsection 2.4.1). If the refractive index is piecewise constant, refraction and reflection at internal interfaces affect photon trajectories but do not introduce any explicit dependence on μ_a or μ_s. Therefore, the same factorization used above still applies: interface effects are included into the coefficients $C_{\mathrm{R}_k}(\ell)$, provided that the total pathlength ℓ is defined as the physical length traveled along the refracted/reflected trajectory. In this convention, interface events are *not* counted as scattering events, so that k retains its meaning as the number of bulk scattering interactions. It may also be useful to recall that Eq. (3) is applicable to both surface-emitting and volume-emitting sources, giving extreme generality to the approach.

Dividing Eq. (3) by $\mathrm{d}\ell$ and summing over all the scattering orders, we obtain the spread function, $\mathrm{SF_R}(\ell)$, for the received power:

$$\mathrm{SF_R}(\ell) = \frac{\mathrm{d}P_\mathrm{R}(\ell)}{\mathrm{d}\ell} = P_\mathrm{E}\mathrm{e}^{-(\mu_\mathrm{a}+\mu_\mathrm{s})\ell}\sum_{k=0}^{+\infty} C_{\mathrm{R}_k}(\ell)\mu_\mathrm{s}^k, \tag{4}$$

with $\mathrm{d}P_\mathrm{R}(\ell) \equiv \sum_{k=0}^{+\infty} \mathrm{d}P_{\mathrm{R}_k}(\ell)$, and where the $k = 0$ term represents the contribution of un-scattered (ballistic) photons. The spread function describes the distribution of pathlengths ℓ traveled within the total volume V of the medium by all received photons.

In a homogeneous medium, with volume V and refractive index n, the time of flight t is simply related to the pathlength ℓ and to the speed of light in vacuum c, by $t = n\ell/c$. This implies that the spread function $\mathrm{SF_R}(\ell)$ is strictly connected to the temporal spread function $\mathrm{TPSF_R}(t)$ by the relation $\mathrm{TPSF_R}(t) = \mathrm{d}P_\mathrm{R}(t)/\mathrm{d}t$; with $P_\mathrm{R}(t)$ representing the power received by the detector at time t. As is well known, $\mathrm{TPSF_R}(t)$ can be experimentally assessed using pulsed sources and time-resolved detection experimental setups [20].

Integrating Eq. (4) over $\mathrm{d}\ell$ we obtain the total received power P_R:

$$P_\mathrm{R} = P_\mathrm{E} \int_0^{+\infty} \mathrm{e}^{-(\mu_\mathrm{a}+\mu_\mathrm{s})\ell} \sum_{k=0}^{+\infty} C_{\mathrm{R}_k}(\ell)\mu_\mathrm{s}^k \mathrm{d}\ell. \tag{5}$$

Equation (5) relates P_R measured in continuous wave (CW) experiments with μ_a and μ_s.

Thus, Eqs. (2) and (3) represent the basic relationships relating the received power to the optical and geometrical parameters of the medium. However, in this form, they are of poor practical use due to the fact that $C_{\mathrm{R}_k}(\ell)$ is in most cases difficult to obtain. In the next section we will see how, thanks to the independence of $C_{\mathrm{R}_k}(\ell)$ from μ_a and μ_s, Eqs. (2), (3) and (5) can be exploited to obtain useful relationships independent from $C_{\mathrm{R}_k}(\ell)$.

Note that the physical meaning of $C_{\mathrm{R}_k}(\ell)$ can be deduced by observing Eq. (3). In fact, $\exp[-(\mu_\mathrm{a} + \mu_\mathrm{s})\ell]$ represents the fraction of remaining power due to absorption and scattering events at the end of a path of length ℓ. The term $\mu_\mathrm{s}\mathrm{d}\ell$ represents the probability to be scattered along a path of length $\mathrm{d}\ell$, at the end of ℓ. Thus, due to the construction of Eq. (3) from Eq. (1) with the meaning given to $\mathrm{d}P_{\mathrm{R}_k}(\ell)$, and using the physical meaning of μ_s, $C_{\mathrm{R}_k}(\ell)\mu_\mathrm{s}^{k-1}$ consistently represents the probability to have exactly k scattering events along ℓ.

It is also important to emphasize that the factorization leading to Eq. (3) does not assume any specific scattering phase function. All dependence on the phase function is included into the coefficients $C_{\mathrm{R}_k}(\ell)$ (and their heterogeneous counterparts), whereas the dependence on μ_a and μ_s appears only through $\mu_\mathrm{s}^k \exp[-(\mu_\mathrm{a} + \mu_\mathrm{s})\ell]$. Consequently, the identities derived here apply to Henyey–Greenstein scattering as well as to arbitrary phase functions.

Furthermore, throughout this work μ_a denotes the macroscopic absorption coefficient experienced by photons along their trajectories. It may represent absorption by the host medium, by dispersed particles, or by any combination thereof; the derivations rely only on its standard radiative-transfer interpretation as an attenuation rate per unit pathlength.

2.1.2. Received power sensitivity on μ_a and μ_s

The received power sensitivity on μ_a and μ_s provides useful information concerning, e.g., the performance of biomedical-optics instrumentation. It is usually obtained by taking the μ_a or μ_s derivative of the logarithm of the parameter of interest. For example, the logarithmic derivative of the total received power is related to measurements in the CW domain while the logarithmic derivative of the spread function is related to measurements in the time domain (TD).

Thus, from Eq. (4) we obtain

$$\frac{\partial \ln(\mathrm{SF_R}(\ell))}{\partial \mu_\mathrm{a}} = -\ell, \tag{6}$$

$$\frac{\partial \ln(\mathrm{SF_R}(\ell))}{\partial \mu_\mathrm{s}} = \frac{P_\mathrm{E}\mathrm{e}^{-(\mu_\mathrm{a}+\mu_\mathrm{s})\ell} \sum_{k=0}^{+\infty} \mu_\mathrm{s}^k \left(-\ell C_{\mathrm{R}_k}(\ell) + k C_{\mathrm{R}_k}(\ell)\mu_\mathrm{s}^{-1}\right)}{P_\mathrm{E}\mathrm{e}^{-(\mu_\mathrm{a}+\mu_\mathrm{s})\ell} \sum_{k=0}^{+\infty} C_{\mathrm{R}_k}(\ell)\mu_\mathrm{s}^k} = \frac{\langle k \rangle_\mathrm{R}(\ell)}{\mu_\mathrm{s}} - \ell, \tag{7}$$

and from Eq. (5) we obtain

$$\frac{\partial \ln(P_\mathrm{R})}{\partial \mu_\mathrm{a}} = \frac{-\int_0^{+\infty} \ell P_\mathrm{E}\mathrm{e}^{-(\mu_\mathrm{a}+\mu_\mathrm{s})\ell} \sum_{k=0}^{+\infty} C_{\mathrm{R}_k}(\ell)\mu_\mathrm{s}^k \mathrm{d}\ell}{\int_0^{+\infty} P_\mathrm{E}\mathrm{e}^{-(\mu_\mathrm{a}+\mu_\mathrm{s})\ell} \sum_{k=0}^{+\infty} C_{\mathrm{R}_k}(\ell)\mu_\mathrm{s}^k \mathrm{d}\ell} = -\langle \ell \rangle_\mathrm{R}, \tag{8}$$

$$\frac{\partial \ln(P_\mathrm{R})}{\partial \mu_\mathrm{s}} = \frac{\int_0^{+\infty} P_\mathrm{E}\mathrm{e}^{-(\mu_\mathrm{a}+\mu_\mathrm{s})\ell} \sum_{k=0}^{+\infty} \mu_\mathrm{s}^k \left(-\ell C_{\mathrm{R}_k}(\ell) + k C_{\mathrm{R}_k}(\ell)\mu_\mathrm{s}^{-1}\right) \mathrm{d}\ell}{\int_0^{+\infty} P_\mathrm{E}\mathrm{e}^{-(\mu_\mathrm{a}+\mu_\mathrm{s})\ell} \sum_{k=0}^{+\infty} C_{\mathrm{R}_k}(\ell)\mu_\mathrm{s}^k \mathrm{d}\ell} = \frac{\langle k \rangle_\mathrm{R}}{\mu_\mathrm{s}} - \langle \ell \rangle_\mathrm{R}. \tag{9}$$

Equation (9) provides an *exact* identity linking the scattering sensitivity of the detected signal to two trajectory statistics of the received photons: $\partial \ln(P_R)/\partial \mu_s = \langle k \rangle_\mathrm{R}/\mu_\mathrm{s} - \langle \ell \rangle_\mathrm{R}$. Naively, one would expect the right-hand side to vanish in the diffusive regime, based on the idea that the number of scattering events should scale as $\mu_s\ell$. However, for received photons this direct proportionality is not exact in general because the detection conditions bias the joint statistics of (k,ℓ). Importantly, if the mismatch $\langle k\rangle_R/\mu_s - \langle\ell\rangle_R$ was in general zero, then $\partial \ln(P_R)/\partial\mu_s = 0$, which would mean that the received signal would be insensitive to μ_s variations.

These expressions show that the sensitivity of the received power to variations of μ_a is only related to the pathlength traveled by received photons: to ℓ itself for the spread function, and to the mean pathlength $\langle\ell\rangle_R$ for CW received power.

Instead, the sensitivity to variations of μ_s is related to both the length of the path traveled and the number of scattering events. The spread function sensitivity is related to ℓ itself and to the mean number of scattering events, $\langle k\rangle_R(\ell)$,

$$\langle k\rangle_R(\ell) = \frac{\sum_{k=0}^{+\infty} k\mu_s^{k-1} C_{R_k}(\ell)}{\sum_{k=0}^{+\infty} \mu_s^{k-1} C_{R_k}(\ell)} = \frac{\mu_s}{\mu_s}\frac{\sum_{k=0}^{+\infty} k\mu_s^{k-1} C_{R_k}(\ell)}{\sum_{k=0}^{+\infty} \mu_s^{k-1} C_{R_k}(\ell)} = \frac{\sum_{k=0}^{+\infty} k\mu_s^{k} C_{R_k}(\ell)}{\sum_{k=0}^{+\infty} \mu_s^{k} C_{R_k}(\ell)}, \tag{10}$$

a term averaged only over received photons with pathlength ℓ. Similarly, the sensitivity of the total received power is related to the mean pathlength $\langle\ell\rangle_R$ and to the total mean number of scattering events, $\langle k\rangle_R$,

$$\langle k\rangle_R = \frac{\sum_{k=0}^{+\infty} k\mu_s^k \int_0^{+\infty} e^{-(\mu_a+\mu_s)\ell} C_{R_k}(\ell)d\ell}{\sum_{k=0}^{+\infty} \mu_s^k \int_0^{+\infty} e^{-(\mu_a+\mu_s)\ell} C_{R_k}(\ell)d\ell}, \tag{11}$$

a term averaged on all received photons.

Since the mean free path traveled between two subsequent scattering events is given by $\ell_s = 1/\mu_s$, we should expect, especially for propagation in the diffusive regime, that $\langle k\rangle_R(\ell)/\mu_s \approx \ell$ and $\langle k\rangle_R/\mu_s \approx \langle\ell\rangle_R$. The exact relations here derived show that this intuitive direct proportionality is not exact for detected/received photons in general. Thus, the sensitivity to variations of the scattering coefficient is significantly lower than for variations of the absorption coefficient. This is perhaps the main reason why, for both TD and CW measurements, the scattering coefficient is usually retrieved with worse precision and accuracy than the absorption coefficient [21,22].

2.2. Homogeneous medium: the absorbed power

Similar relations to those obtained for the received power can also be obtained for the absorbed power.

2.2.1. Basic relationships

The power absorbed in a volume element of thickness $d\ell$ is equal to $\mu_a d\ell$ times the incident power (see Fig. 2). Thus, the fraction of the emitted power dP_E, along the initial direction of propagation $\hat{\mathbf{s}}_0$, that is absorbed by the volume element of thickness $d\ell_A$, after having traveled the trajectory with k scattering events, can be written as

$$d\tilde{P}_{A_k} = dP_E\mu_s^k e^{-(\mu_a+\mu_s)\ell} \prod_{i=1}^{k} [d\ell_i p(\hat{\mathbf{s}}_i, \hat{\mathbf{s}}_{i-1})d\hat{\mathbf{s}}_i]\, \mu_a d\ell_A. \tag{12}$$

The total absorbed power, after having traveled trajectories with k scattering events and a total length between ℓ and $\ell + d\ell$, can be obtained by adding all the possible $d\tilde{P}_{A_k}$ contributions of the trajectories space, as

$$dP_{A_k} = P_E C_{A_k}(\ell)\mu_a\mu_s^k e^{-(\mu_a+\mu_s)\ell} d\ell, \tag{13}$$

and the relationships for the spread function of the absorbed power, $SF_A(\ell)$, and for the total absorbed power P_A, can be written as:

$$SF_A(\ell) = \frac{dP_A(\ell)}{d\ell} = P_E\mu_a e^{-(\mu_a+\mu_s)\ell} \sum_{k=0}^{+\infty} C_{A_k}(\ell)\mu_s^k, \tag{14}$$

$$P_{\mathrm{A}} = P_{\mathrm{E}} \int_0^{\infty} \mu_{\mathrm{a}} \mathrm{e}^{-(\mu_{\mathrm{a}}+\mu_{\mathrm{s}})\ell} \sum_{k=0}^{+\infty} C_{\mathrm{A}_k}(\ell)\mu_{\mathrm{s}}^k \mathrm{d}\ell, \tag{15}$$

where it is worth noting the formal similitude (up to a multiplicative constant μ_{a}) of the relations for the absorbed power (Eqs. (13) to (15)) with those for the received power (Eqs. (3) to (5)).

These expressions can be applicable both to the power absorbed in the whole volume and to the power absorbed in any sub-volume $\overline{V} \subseteq V$. This implies that the coefficients $C_{\mathrm{A}_k}(\ell)$ will depend on the considered $\overline{V}$.

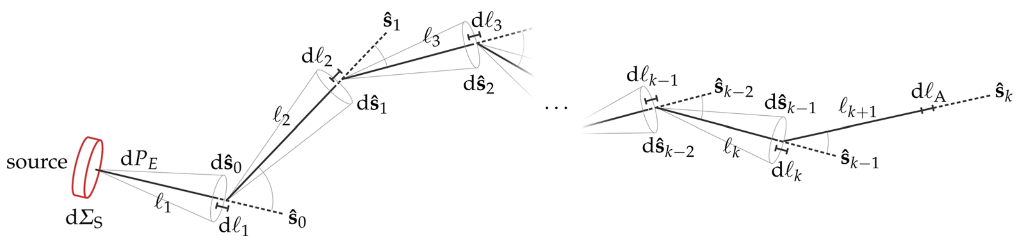

Fig. 2. Example of trajectory with k scattering events traveled by the emitted power $\mathrm{d}P_{\mathrm{E}}$ to reach the volume element $\mathrm{d}\ell_{\mathrm{A}}$.

2.2.2. Absorbed power sensitivity on μ_{a} and μ_{s}

Similarly to Subsection 2.1.2, by using Eqs. (14) and (15), the logarithmic derivatives — giving the sensitivity to μ_{a} and μ_{s} of the different parameters — can also be obtained for the absorbed power.

Thus, from Eq. (14) we obtain

$$\frac{\partial \ln(\mathrm{SF}_{\mathrm{A}}(\ell))}{\partial \mu_{\mathrm{a}}} = \frac{1}{\mu_{\mathrm{a}}} - \ell, \tag{16}$$

$$\frac{\partial \ln(\mathrm{SF}_{\mathrm{A}}(\ell))}{\partial \mu_{\mathrm{s}}} = \frac{\langle k \rangle_{\mathrm{A}}(\ell)}{\mu_{\mathrm{s}}} - \ell, \tag{17}$$

and from Eq. (15) we obtain

$$\frac{\partial \ln(P_{\mathrm{A}})}{\partial \mu_{\mathrm{a}}} = \frac{1}{\mu_{\mathrm{a}}} - \langle \ell \rangle_{\mathrm{A}}, \tag{18}$$

$$\frac{\partial \ln(P_{\mathrm{A}})}{\partial \mu_{\mathrm{s}}} = \frac{\langle k \rangle_{\mathrm{A}}}{\mu_{\mathrm{s}}} - \langle \ell \rangle_{\mathrm{A}}. \tag{19}$$

The derivatives with respect to μ_{s} are identical to those of the received power. Those with respect to μ_{a} are instead significantly different especially for small values of absorption, since the term $1/\mu_{\mathrm{a}}$ can become very large.

2.3. *Homogeneous medium: the total power*

In Subsection 2.1.1 a relationship for the dependence of P_{R} on μ_{a} and μ_{s} coefficients has been described. In Subsection 2.1.2, the corresponding expressions for the sensitivity of P_{R} on μ_{a} and μ_{s} have also been presented. Analogous relationships for P_{A} in a volume $\overline{V} \subseteq V$ have been described in Subsection 2.2.

These identities have been obtained in all generality and are applicable: 1) irrespective of the type and geometry of sources (pulsed or continuous, surface or volume sources located inside and/or outside V); 2) irrespective of the detector for the received power (extension, field of view, inside or outside V) and; 3) for any arbitrary volume $\overline{V}$ for the absorbed power.

The formal relationships for P_{R} are therefore also applicable to a hypothetical detector which envelops the entire volume (capable of detecting all the radiation escaping from V, whatever the position and the direction), and those for P_{A} are also applicable to the total power absorbed over the entire volume V, i.e., for $\overline{V} = V$.

Thus, indicating with $P_{\mathrm{R}}^{\mathrm{T}}$ the total power received by this hypothetical detector and with $P_{\mathrm{A}}^{\mathrm{T}}$ the total power absorbed in V, the energy conservation law allows us to write

$$P_{\mathrm{R}}^{\mathrm{T}} + P_{\mathrm{A}}^{\mathrm{T}} = P_{\mathrm{E}}, \tag{20}$$

where P_{E} is the total power emitted by the sources, which is obviously independent of μ_{a} and μ_{s}.

2.3.1. Fraction of absorbed power and mean pathlength

By expressing the P_{E} sensitivity on μ_{a} and by using Eqs. (8), (18) and (20), we obtain

$$\frac{\partial \ln(P_{\mathrm{E}})}{\partial \mu_{\mathrm{a}}} = \frac{P_{\mathrm{R}}^{\mathrm{T}} \frac{\partial \ln P_{\mathrm{R}}^{\mathrm{T}}}{\partial \mu_{\mathrm{a}}} + P_{\mathrm{A}}^{\mathrm{T}} \frac{\partial \ln P_{\mathrm{A}}^{\mathrm{T}}}{\partial \mu_{\mathrm{a}}}}{P_{\mathrm{E}}} = \frac{-P_{\mathrm{R}}^{\mathrm{T}} \langle \ell \rangle_{\mathrm{R}}^{\mathrm{T}} + P_{\mathrm{A}}^{\mathrm{T}} \left(\frac{1}{\mu_{\mathrm{a}}} - \langle \ell \rangle_{\mathrm{A}}^{\mathrm{T}} \right)}{P_{\mathrm{E}}} = \frac{1}{\mu_{\mathrm{a}}} \frac{P_{\mathrm{A}}^{\mathrm{T}}}{P_{\mathrm{E}}} - \langle \ell \rangle_{\mathrm{E}}^{\mathrm{T}} = 0, \tag{21}$$

where $\langle \ell \rangle_{\mathrm{R}}^{\mathrm{T}}$, $\langle \ell \rangle_{\mathrm{A}}^{\mathrm{T}}$ and $\langle \ell \rangle_{\mathrm{E}}^{\mathrm{T}}$ are the mean pathlengths traveled by the total received power, the total absorbed power, and the total emitted power, respectively. Equation (21) can be rewritten as

$$\frac{P_{\mathrm{A}}^{\mathrm{T}}}{P_{\mathrm{E}}} = \mu_{\mathrm{a}} \langle \ell \rangle_{\mathrm{E}}^{\mathrm{T}}; \tag{22}$$

giving the exact relationship existing between the fraction of total absorbed power and the total mean pathlength.

2.3.2. Mean pathlength and mean number of scattering events

By expressing the P_{E} sensitivity on μ_{s} and by using Eqs. (9), (19) and (20), we obtain

$$\frac{\partial \ln(P_{\mathrm{E}})}{\partial \mu_{\mathrm{s}}} = \frac{P_{\mathrm{R}}^{\mathrm{T}} \frac{\partial \ln P_{\mathrm{R}}^{\mathrm{T}}}{\partial \mu_{\mathrm{s}}} + P_{\mathrm{A}}^{\mathrm{T}} \frac{\partial \ln P_{\mathrm{A}}^{\mathrm{T}}}{\partial \mu_{\mathrm{s}}}}{P_{\mathrm{E}}} = \frac{-P_{\mathrm{R}}^{\mathrm{T}} \left(\frac{\langle k \rangle_{\mathrm{R}}^{\mathrm{T}}}{\mu_{\mathrm{s}}} - \langle \ell \rangle_{\mathrm{R}}^{\mathrm{T}} \right) + P_{\mathrm{A}}^{\mathrm{T}} \left(\frac{\langle k \rangle_{\mathrm{A}}^{\mathrm{T}}}{\mu_{\mathrm{s}}} - \langle \ell \rangle_{\mathrm{A}}^{\mathrm{T}} \right)}{P_{\mathrm{E}}} = \frac{\langle k \rangle_{\mathrm{E}}^{\mathrm{T}}}{\mu_{\mathrm{s}}} - \langle \ell \rangle_{\mathrm{E}}^{\mathrm{T}} = 0, \tag{23}$$

where $\langle k \rangle_{\mathrm{R}}^{\mathrm{T}}$, $\langle k \rangle_{\mathrm{A}}^{\mathrm{T}}$ and $\langle k \rangle_{\mathrm{E}}^{\mathrm{T}}$ are the mean number of scattering events undergone by the total received power, the total absorbed power, and the total emitted power, respectively. This equation can be rewritten as

$$\frac{\langle k \rangle_{\mathrm{E}}^{\mathrm{T}}}{\mu_{\mathrm{s}}} = \langle \ell \rangle_{\mathrm{E}}^{\mathrm{T}}, \tag{24}$$

establishing an exact relationship between the mean pathlength and the mean number of scattering events for the total emitted power.

Equation (24) is true only if one considers the total number of scattering events of the emitted power that can be both absorbed or received. An important contribution to $\langle k \rangle_{\mathrm{E}}^{\mathrm{T}}$ is thus also given by the scattering events undergone by the absorbed light before being extinguished. On the contrary to what one might intuitively think, a relationship similar to Eq. (24) is not true when considering only the received power, i.e., using $\langle k \rangle_{\mathrm{R}}^{\mathrm{T}}$ and $\langle \ell \rangle_{\mathrm{R}}^{\mathrm{T}}$ instead of $\langle k \rangle_{\mathrm{E}}^{\mathrm{T}}$ and $\langle \ell \rangle_{\mathrm{E}}^{\mathrm{T}}$ with the sole exception of a completely non-absorbing medium for which $\langle k \rangle_{\mathrm{R}}^{\mathrm{T}} = \langle k \rangle_{\mathrm{E}}^{\mathrm{T}}$ and $\langle \ell \rangle_{\mathrm{R}}^{\mathrm{T}} = \langle \ell \rangle_{\mathrm{E}}^{\mathrm{T}}$.

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2.3.3. Fraction of absorbed power and mean number of scattering events

Combining Eqs. (22) and (24) the fraction of absorbed power can also be expressed as

$$\frac{P_{\mathrm{A}}^{\mathrm{T}}}{P_{\mathrm{E}}} = \frac{\mu_{\mathrm{a}}}{\mu_{\mathrm{s}}}\langle k\rangle_{\mathrm{E}}^{\mathrm{T}}. \tag{25}$$

Equation (25) represents an exact relationship between the total absorbed power and the mean number of scattering events undergone by the total emitted power.

2.4. *Heterogeneous medium: the received power*

2.4.1. Basic relationships

Let us consider a non-homogeneous medium with volume V and light sources and detectors distributed as in Subsection 2.1.1. The medium is divided of M sub-volumes V_i, with $i = 1, \ldots, M$. Each V_i has uniform absorption and scattering coefficients, $\mu_{\mathrm{a},i}$ and $\mu_{\mathrm{s},i}$, and refractive index n_i (see Fig. 3). We are interested in the relationship existing between the received power and $\mu_{\mathrm{a},i}$ and $\mu_{\mathrm{s},i}$ of a sub-volume V_i. By following the same reasoning used for the homogeneous medium (Subsection 2.1.1), the total power $\mathrm{d}P_{\mathrm{R}_{k,i}}(\ell_i)$ received by trajectories with a total length spent inside V_i between ℓ_i and $\ell_i + \mathrm{d}\ell_i$ and k scattering events, occurred only in V_i, can be expressed as:

$$\mathrm{d}P_{\mathrm{R}_{k,i}}(\ell_i) = P_{\mathrm{E}} C_{\mathrm{R}_{k,i}}(\ell_i)\, \mu_{\mathrm{s},i}^{k} \mathrm{e}^{-(\mu_{\mathrm{a},i}+\mu_{\mathrm{s},i})\ell_i} \mathrm{d}\ell_i, \tag{26}$$

where $C_{\mathrm{R}_{k,i}}(\ell_i)$ is a coefficient which depends on ℓ_i and on many other factors such as source and receiver geometries, geometry of the medium, scattering functions and, internal and external refractive indexes. Last but not least, $C_{\mathrm{R}_{k,i}}(\ell_i)$ also depends on $\mu_{\mathrm{a},j}$ and $\mu_{\mathrm{s},j}$ of sub-volumes V_j, with $j \neq i$. However, $C_{\mathrm{R}_{k,i}}(\ell_i)$ does not depend on $\mu_{\mathrm{a},i}$ and $\mu_{\mathrm{s},i}$.

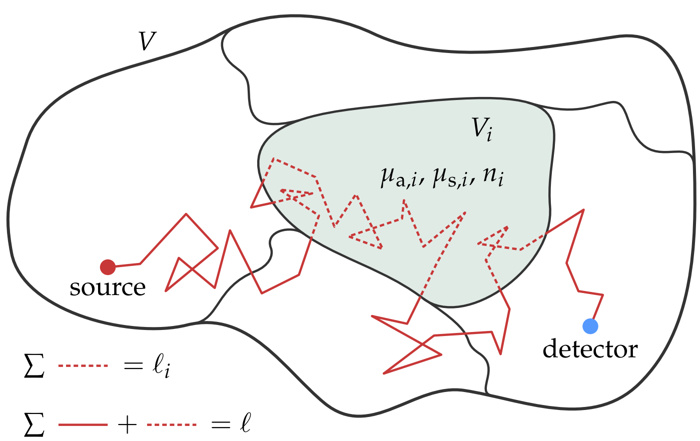

Fig. 3. Schematic depiction of a heterogeneous domain with volume V and with sub-domains (here we show only 5 possible sub-domains). In red, an example of a possible trajectory with a volume source and a volume detector.

Dividing Eq. (26) by $\mathrm{d}\ell_i$ and summing over all scattering orders we obtain the spread function, $\mathrm{SF}_{\mathrm{R}_i}(\ell_i)$, for the distribution of pathlengths ℓ_i, traveled only inside V_i, by all the received photons, as

$$\mathrm{SF}_{\mathrm{R}_i}(\ell_i) = \frac{\mathrm{d}P_{\mathrm{R}_i}(\ell_i)}{\mathrm{d}\ell_i} = P_{\mathrm{E}} \mathrm{e}^{-(\mu_{\mathrm{a},i}+\mu_{\mathrm{s},i})\ell_i} \sum_{k=0}^{+\infty} C_{\mathrm{R}_{k,i}}(\ell_i)\mu_{\mathrm{s},i}^{k}, \tag{27}$$

with $\mathrm{d}P_{\mathrm{R}_i}(\ell_i) \equiv \sum_{k=0}^{+\infty} \mathrm{d}P_{\mathrm{R}_{k,i}}(\ell_i)$. It is useful to point out that in $\mathrm{SF}_{\mathrm{R}_i}(\ell_i)$ is also implicitly included a term $\delta(\ell_i)$, taking into contributions of photons received without having intersected V_i, i.e., with $\ell_i = 0$. Integrating Eq. (27) over $\mathrm{d}\ell_i$, the formal expression for the dependence of the total received power on $\mu_{a,i}$ and $\mu_{s,i}$ is obtained

$$P_{R_i} = P_E \int_0^{+\infty} e^{-(\mu_{a,i}+\mu_{s,i})\ell_i} \sum_{k=0}^{+\infty} C_{R_{k,i}}(\ell_i)\mu_{s,i}^k \mathrm{d}\ell_i. \tag{28}$$

This is a relationship between the total received power and the scattering and absorption coefficients of the sub-volume V_i.

2.4.2. Received power sensitivity on $\mu_{a,i}$ and $\mu_{s,i}$

From the logarithmic derivatives of Eq. (27), we obtain

$$\frac{\partial \ln(\mathrm{SF}_{R_i}(\ell_i))}{\partial \mu_{a,i}} = -\ell_i, \tag{29}$$

$$\frac{\partial \ln(\mathrm{SF}_{R_i}(\ell_i))}{\partial \mu_{s,i}} = \frac{\langle k\rangle_{R,i}(\ell_i)}{\mu_{s,i}} - \ell_i, \tag{30}$$

and from the logarithmic derivatives of Eq. (28), we obtain

$$\frac{\partial \ln(P_{R_i})}{\partial \mu_{a,i}} = -\langle \ell_i\rangle_R, \tag{31}$$

$$\frac{\partial \ln(P_{R_i})}{\partial \mu_{s,i}} = \frac{\langle k\rangle_{R,i}}{\mu_{s,i}} - \langle \ell_i\rangle_R, \tag{32}$$

where $\langle k\rangle_{R,i}(\ell_i)$ is the mean number of scattering events undergone by received photons that traveled the pathlength ℓ_i within V_i and, $\langle \ell_i\rangle_R$ and $\langle k\rangle_{R,i}$ are the mean pathlength and the average number of scattering events within V_i for the total received photons, respectively.

For the non-homogeneous medium, the logarithmic derivatives describe the relative change in received power due to localized variations in the optical properties, i.e. the sensitivity of received power to local variations of μ_a and μ_s. They are therefore the Jacobians used for image reconstruction in diffuse optical tomography (DOT) [23,24].

Also for the non-homogeneous medium, we in general expect that $\langle k\rangle_{R,i}(\ell_i)/\mu_{s,i} \approx \ell_i$ and $\langle k\rangle_{R,i}/\mu_{s,i} \approx \langle \ell_i\rangle_R$, for which the sensitivity to local variations of $\mu_{s,i}$ is expected to be significantly lower than that for variations of $\mu_{a,i}$.

2.5. Heterogeneous medium: the absorbed power

Even in the heterogeneous case, similar relations to those obtained for the received power (Subsection 2.4) can also be obtained for the absorbed power.

2.5.1. Basic relationships

To write the relationship for the total power, $\mathrm{d}P_{\bar{A}_{k,i}}(\ell_i)$, absorbed within a volume $\overline{V} \subseteq V$ after having traveled trajectories with a total length ℓ_i and a number k of scattering events within the sub-volume V_i (see Fig. 4), it is necessary to distinguish the fraction of $\mathrm{d}P_{\bar{A}_{k,i}}(\ell_i)$ absorbed within V_i itself, $\mathrm{d}P_{A^*_{k,i}}(\ell_i)$, from the fraction of $\mathrm{d}P_{\bar{A}_{k,i}}(\ell_i)$ absorbed within $V^\dagger = \overline{V} \setminus V_i$, i.e., $\mathrm{d}P_{A^\dagger_{k,i}}(\ell_i)$. Thus $\mathrm{d}P_{\bar{A}_{k,i}}(\ell_i)$ can be written as

$$\mathrm{d}P_{\bar{A}_{k,i}}(\ell_i) = \mathrm{d}P_{A^*_{k,i}}(\ell_i) + \mathrm{d}P_{A^\dagger_{k,i}}(\ell_i). \tag{33}$$

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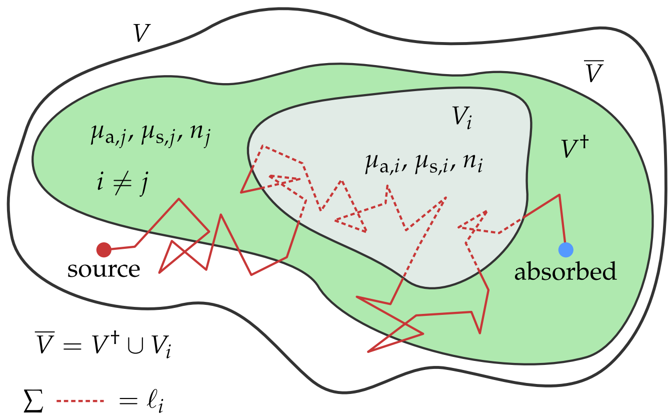

Fig. 4. Schematic depiction of a heterogeneous domain V with absorbing sub-domains $\overline{V}$ and V_i, with $V_i \subseteq \overline{V}$.

Obviously, if $V_i \not\subset \overline{V}$ then $\mathrm{d}P_{\mathrm{A}^*_{k,i}}(\ell_i) = 0$. For the power $\mathrm{d}P_{\mathrm{A}^*_{k,i}}(\ell_i)$ absorbed within V_i the dependence on $\mu_{\mathrm{a},i}$ and $\mu_{\mathrm{s},i}$ is

$$\mathrm{d}P_{\mathrm{A}^*_{k,i}}(\ell_i) = P_\mathrm{E} C_{\mathrm{A}^*_{k,i}}(\ell_i)\, \mu_{\mathrm{a},i}\mu^k_{\mathrm{s},i}\mathrm{e}^{-(\mu_{\mathrm{a},i}+\mu_{\mathrm{s},i})\ell_i}\mathrm{d}\ell_i, \tag{34}$$

and for $\mathrm{d}P_{\mathrm{A}^\dagger_{k,i}}(\ell_i)$ is

$$\mathrm{d}P_{\mathrm{A}^\dagger_{k,i}}(\ell_i) = P_\mathrm{E} C_{\mathrm{A}^\dagger_{k,i}}(\ell_i)\, \mu^k_{\mathrm{s},i}\mathrm{e}^{-(\mu_{\mathrm{a},i}+\mu_{\mathrm{s},i})\ell_i}\mathrm{d}\ell_i. \tag{35}$$

The derivation of Eq. (34) is straightforward and similar to the procedure used for the received power, thus the coefficient $C_{\mathrm{A}^*_{k,i}}(\ell_i)$ has similar meaning and same units of the coefficient $C_{\mathrm{R}_{k,i}}(\ell_i)$ of Eq. (26). However, Eq. (35) shows a different form compared to Eq. (26), since the coefficient $C_{\mathrm{A}^\dagger_{k,i}}(\ell_i)$ also takes into account the effects of absorption and scattering terms external to V_i in order to separate this functional dependence in the overall expression from that relating to the optical properties in V_i. In contrast, $C_{\mathrm{A}^*_{k,i}}(\ell_i)$ does not include the dependence of any absorption or scattering. Thus, in Eq. (34), the dependence on absorption and scattering appears only in the term $\mu_{\mathrm{a},i}\mu^k_{\mathrm{s},i}\,\mathrm{e}^{-(\mu_{\mathrm{a},i}+\mu_{\mathrm{s},i})\ell_i}$. Therefore, $C_{\mathrm{A}^\dagger_{k,i}}(\ell_i)$ is also a function of $\mu_{\mathrm{a},j}$ and $\mu_{\mathrm{s},j}$ with $j \neq i$ (see Fig. 4). This fact implies that $C_{\mathrm{A}^\dagger_{k,i}}(\ell_i)$ has different units compared to $C_{\mathrm{A}^*_{k,i}}(\ell_i)$, accordingly to the meaning of Eq. (35).

Dividing Eqs. (34) and (35) by $\mathrm{d}\ell_i$ and summing over all the scattering orders k we obtain the expressions for the spread functions:

$$\mathrm{SF}_{\mathrm{A}^*_i}(\ell_i) = P_\mathrm{E}\mu_{\mathrm{a},i}\mathrm{e}^{-(\mu_{\mathrm{a},i}+\mu_{\mathrm{s},i})\ell_i}\sum_{k=0}^{\infty} C_{\mathrm{A}^*_{k,i}}(\ell_i)\mu^k_{\mathrm{s},i}, \tag{36}$$

$$\mathrm{SF}_{\mathrm{A}^\dagger_i}(\ell_i) = P_\mathrm{E}\mathrm{e}^{-(\mu_{\mathrm{a},i}+\mu_{\mathrm{s},i})\ell_i}\sum_{k=0}^{\infty} C_{\mathrm{A}^\dagger_{k,i}}(\ell_i)\mu^k_{\mathrm{s},i}. \tag{37}$$

The spread function for the total absorbed power within the volume $\overline{V}$, $\mathrm{SF}_{\bar{\mathrm{A}}_i}(\ell_i)$, is obtained by adding Eqs. (36) and (37):

$$\mathrm{SF}_{\bar{\mathrm{A}}_i}(\ell_i) = \mathrm{SF}_{\mathrm{A}^*_i}(\ell_i) + \mathrm{SF}_{\mathrm{A}^\dagger_i}(\ell_i) = P_\mathrm{E}\mathrm{e}^{-(\mu_{\mathrm{a},i}+\mu_{\mathrm{s},i})\ell_i}\sum_{k=0}^{\infty}\mu^k_{\mathrm{s},i}\left(\mu_{\mathrm{a},i}C_{\mathrm{A}^*_{k,i}}(\ell_i) + C_{\mathrm{A}^\dagger_{k,i}}(\ell_i)\right). \tag{38}$$

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By integrating Eq. (38) over $d\ell_i$, we obtain the formal expression for the dependence of total absorbed power on $\mu_{a,i}$ and $\mu_{s,i}$, i.e.:

$$P_{\bar{A}_i} = P_{A_i^*} + P_{A_i^\dagger} = \int_0^\infty P_E e^{-(\mu_{a,i}+\mu_{s,i})\ell_i} \sum_{k=0}^\infty \mu_{s,i}^k \left(\mu_{a,i} C_{A_{k,i}^*}(\ell_i) + C_{A_{k,i}^\dagger}(\ell_i)\right) d\ell_i. \tag{39}$$

2.5.2. Absorbed power sensitivity on $\mu_{a,i}$ and $\mu_{s,i}$

Let us take into account the fact that $C_{A_{k,i}^*}(\ell_i)$ and $C_{A_{k,i}^\dagger}(\ell_i)$ do not depend on $\mu_{a,i}$ and $\mu_{s,i}$ (see Subsection 2.5.1). Thus, by making the logarithmic derivative with respect to $\mu_{a,i}$ and $\mu_{s,i}$ of Eq. (38) — for the spread function of the power absorbed in a sub-volume $\overline{V} \subseteq V$ (see Fig. 4) — we obtain

$$\frac{\partial \ln(\mathrm{SF}_{\bar{A}_i}(\ell_i))}{\partial \mu_{a,i}} = \frac{1}{\mu_{a,i}} \frac{\mathrm{SF}_{A_i^*}(\ell_i)}{\mathrm{SF}_{\bar{A}_i}(\ell_i)} - \ell_i, \tag{40}$$

$$\frac{\partial \ln(\mathrm{SF}_{\bar{A}_i}(\ell_i))}{\partial \mu_{s,i}} = \frac{\langle k\rangle_{A,i}(\ell_i)}{\mu_{s,i}} - \ell_i, \tag{41}$$

where $\langle k\rangle_{A,i}(\ell_i)$ is the mean number of scattering events undergone within V_i by photons absorbed in $\overline{V}$, after traveling the pathlength ℓ_i.

By making the logarithmic derivative with respect to $\mu_{a,i}$ and $\mu_{s,i}$ of the total power $P_{\bar{A}_i}$ (Eq. (39)), absorbed in a volume $\overline{V} \subseteq V$, we obtain

$$\frac{\partial \ln(P_{\bar{A}_i})}{\partial \mu_{a,i}} = \frac{1}{\mu_{a,i}} \frac{P_{A_i^*}}{P_{\bar{A}_i}} - \langle \ell_i\rangle_A, \tag{42}$$

$$\frac{\partial \ln(P_{\bar{A}_i})}{\partial \mu_{s,i}} = \frac{\langle k\rangle_{A,i}}{\mu_{s,i}} - \langle \ell_i\rangle_A, \tag{43}$$

where $P_{A_i^*}$ is the fraction of $P_{\bar{A}_i}$ absorbed in V_i and, $\langle \ell_i\rangle_A$ and $\langle k\rangle_{A,i}$ are respectively the mean pathlength and the mean scattering number, within V_i.

If the sub-volume V_i is external to $\overline{V}$, i.e., $V_i \subset V \setminus \overline{V}$, being $\mathrm{SF}_{\bar{A}_i}(\ell_i) = 0$ and $P_{\bar{A}_i} = 0$, the relationships for the logarithmic derivatives of the absorbed power became identical to the corresponding relations for the received power.

2.6. Heterogeneous medium: the total power

Similarly to Subsection 2.3, we consider a detector capable of detecting all the radiation escaping from V, whatever the position and the direction, which then envelops V. We also impose that the total power is absorbed by all the volume V, i.e., $\overline{V} = V$. This means that the total power received and absorbed is equal to the emitted power and

$$P_{R_i}^T + P_{A_i}^T = P_{E_i}^T = P_E, \tag{44}$$

where $P_{R_i}^T$ is the total power received by the detector and $P_{A_i}^T$ the total power absorbed in V. In the following sections, as for the homogeneous medium, exact relationships linking the absorbed power to the mean path traveled by all the emitted photons and to the mean number of scattering undergone are obtained from the logarithmic derivatives of P_E.

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2.6.1. Fraction of absorbed power and mean pathlength

From the logarithmic derivative of Eq. (44) with respect to $\mu_{a,i}$ and by using Eqs. (31) and (42) with the condition $\overline{V} = V$, we obtain

$$\frac{\partial \ln(P_E)}{\partial \mu_{a,i}} = \frac{P^T_{R_i}\frac{\partial \ln P^T_{R_i}}{\partial \mu_{a,i}} + P^T_{A_i}\frac{\partial \ln P^T_{A_i}}{\partial \mu_{a,i}}}{P_E} = \frac{-P^T_{R_i}\langle \ell_i\rangle^T_R + P^T_{A_i}\left(\frac{1}{\mu_{a,i}}\frac{P^T_{A^*_i}}{P^T_{A_i}} - \langle \ell_i\rangle^T_A\right)}{P_E} = \frac{1}{\mu_{a,i}}\frac{P^T_{A^*_i}}{P_E} - \langle \ell_i\rangle^T_E = 0, \tag{45}$$

where $P^T_{A^*_i}$ is the power absorbed within V_i and, $\langle \ell_i\rangle^T_R$, $\langle \ell_i\rangle^T_A$ and $\langle \ell_i\rangle^T_E$ are the mean pathlengths traveled in V_i by the total received power $P^T_{R_i}$, by the total absorbed power $P^T_{A_i}$, and by the total emitted power P_E, respectively. From Eq. (45) we obtain the following exact relationship between the power absorbed in V_i and the total mean pathlength traveled in V_i:

$$\frac{P^T_{A^*_i}}{P_E} = \mu_{a,i}\langle \ell_i\rangle^T_E. \tag{46}$$

2.6.2. Mean pathlength and mean number of scattering events

From the logarithmic derivative of Eq. (44) with respect to $\mu_{s,i}$ and by using Eqs. (32) and (43), we obtain

$$\frac{\partial \ln(P_E)}{\partial \mu_{s,i}} = \frac{P^T_{R_i}\frac{\partial \ln P^T_{R_i}}{\partial \mu_{s,i}} + P^T_{A_i}\frac{\partial \ln P^T_{A_i}}{\partial \mu_{s,i}}}{P_E} = \frac{-P^T_{R_i}\left(\frac{\langle k\rangle^T_{R,i}}{\mu_{s,i}} - \langle \ell_i\rangle^T_R\right) + P^T_{A_i}\left(\frac{\langle k\rangle^T_{A,i}}{\mu_{s,i}} - \langle \ell_i\rangle^T_A\right)}{P_E} = \frac{\langle k\rangle^T_{E,i}}{\mu_{s,i}} - \langle \ell_i\rangle^T_E = 0, \tag{47}$$

where $\langle k\rangle^T_{R,i}$, $\langle k\rangle^T_{A,i}$, and $\langle k\rangle^T_{E,i}$ are the mean number of scattering undergone in V_i for $P^T_{R_i}$, $P^T_{A_i}$ and P_E, respectively. From this equation the following exact relationship between the mean pathlength traveled in V_i and the mean number of scattering undergone in V_i by the total emitted power is obtained, as

$$\frac{\langle k\rangle^T_{E,i}}{\mu_{s,i}} = \langle \ell_i\rangle^T_E. \tag{48}$$

2.6.3. Fraction of absorbed power and mean number of scattering events

From Eqs. (46) and (48) the fraction of power absorbed in V_i can be also expressed as

$$\frac{P^T_{A^*_i}}{P_E} = \frac{\mu_{a,i}}{\mu_{s,i}}\langle k\rangle^T_{E,i}. \tag{49}$$

The fraction of power absorbed in V_i is therefore strictly connected also to the mean number of scattering events in V_i.

2.6.4. Relations taking into account all sub-sets of *V*

Summing Eqs. (46), (48) and (49) — obtained for the generic sub-volume V_i — over all the M sub-volumes in which can be decomposed V, we finally can express the corresponding relationships for the total volume:

$$\frac{P_{\mathrm{A}}^{\mathrm{T}}}{P_{\mathrm{E}}} = \sum_{i=1}^{M} \frac{P_{\mathrm{A}_i^*}^{\mathrm{T}}}{P_{\mathrm{E}}} = \sum_{i=1}^{M} \mu_{\mathrm{a},i} \langle \ell_i \rangle_{\mathrm{E}}^{\mathrm{T}}, \tag{50}$$

$$\langle k \rangle_{\mathrm{E}}^{\mathrm{T}} = \sum_{i=1}^{M} \langle k \rangle_{\mathrm{E},i}^{\mathrm{T}} = \sum_{i=1}^{M} \mu_{\mathrm{s},i} \langle \ell_i \rangle_{\mathrm{E}}^{\mathrm{T}}, \tag{51}$$

$$\frac{P_{\mathrm{A}}^{\mathrm{T}}}{P_{\mathrm{E}}} = \sum_{i=1}^{M} \frac{P_{\mathrm{A}_i^*}^{\mathrm{T}}}{P_{\mathrm{E}}} = \sum_{i=1}^{M} \frac{\mu_{\mathrm{a},i}}{\mu_{\mathrm{s},i}} \langle k \rangle_{\mathrm{E},i}^{\mathrm{T}}. \tag{52}$$

These relationships hold irrespective of the values of $\mu_{\mathrm{a},i}$ and $\mu_{\mathrm{s},i}$.

For a medium with homogeneous absorption, i.e., $\mu_{\mathrm{a},i} = \mu_{\mathrm{a}}; \forall i \in \{1, 2, \ldots, M\}$, Eq. (50) becomes

$$\frac{P_{\mathrm{A}}^{\mathrm{T}}}{P_{\mathrm{E}}} = \sum_{i=1}^{M} \mu_{\mathrm{a},i} \langle \ell_i \rangle_{\mathrm{E}}^{\mathrm{T}} = \mu_{\mathrm{a}} \langle \ell \rangle_{\mathrm{E}}^{\mathrm{T}}, \tag{53}$$

identical to Eq. (22), and for a medium with homogeneous absorption and scattering coefficients, i.e., $\mu_{\mathrm{s},i} = \mu_{\mathrm{s}}\ \forall i \in \{1, 2, \ldots, M\}$, Eq. (52) becomes

$$\frac{P_{\mathrm{A}}^{\mathrm{T}}}{P_{\mathrm{E}}} = \sum_{i=1}^{M} \frac{\mu_{\mathrm{a},i}}{\mu_{\mathrm{s},i}} \langle k \rangle_{\mathrm{E},i}^{\mathrm{T}} = \frac{\mu_{\mathrm{a}}}{\mu_{\mathrm{s}}} \langle k \rangle_{\mathrm{E}}^{\mathrm{T}}, \tag{54}$$

that is identical to Eq. (25), as expected. Equations (53) and (54) represent also a consistency check between the results for the heterogeneous and homogeneous medium, confirming that the latter is recovered as a special case of the former.

The relationships obtained in this section — concerning the absorbed power *vs.* the mean optical path length and the mean scattering number — establish a sort of equivalence between $P_{\mathrm{A}_i^*}^{\mathrm{T}}/P_{\mathrm{E}}$, $\langle \ell_i \rangle_{\mathrm{E}}^{\mathrm{T}}$ and $\langle k \rangle_{\mathrm{E},i}^{\mathrm{T}}$, since the knowledge of one of these quantities, together with the absorption and scattering coefficients of the medium, allows us to uniquely derive the other two according to Eqs. (48) and (49).

2.7. "Adding scattering" method

The formal expressions for the logarithmic derivatives of the spread functions, $\mathrm{SF}_{\mathrm{R}}(\ell)$ and $\mathrm{SF}_{\mathrm{R}_i}(\ell)$, and of the total received powers, P_{R} and P_{R_i}, with respect to μ_{a} (Eqs. (6), (8), (29) and (31)) provide the foundation for the so-called "Adding absorption" method [25–29]. This method has been used in the past to determine the average path traveled by the received radiation both in laboratory experiments [30–33] and with MC simulations [31,32,34]. This method has also been used to determine the optical properties of diffusive liquids especially for the calibration of fat emulsions such as Intralipid [21,29].

By analogy, the logarithmic derivative with respect to μ_{s} — of the spread functions, $\mathrm{SF}_{\mathrm{R}}(\ell)$ and $\mathrm{SF}_{\mathrm{R}_i}(\ell)$, and of the total received powers, P_{R} and P_{R_i} — allows us to define the "Adding scattering" method, where the logarithmic derivatives express a relation between the mean number of scattering events and the mean path length (Eqs. (7), (9), (30) and (32)). The use of this method in applied fields remains largely unexplored.

For instance, contrary to what one may expect intuitively, the difference $\langle k \rangle_{\mathrm{R}}/\mu_{\mathrm{s}} - \langle \ell \rangle_{\mathrm{R}}$, related to the received power (Eq. (9)), is small but not nil (Subsection 2.1.2). The "Adding scattering" method provides a practical estimation strategy of this difference by means of $\partial \ln(P_{\mathrm{R}})/\partial \mu_{\mathrm{s}}$. In fact, in the CW domain, P_{R} can be obtained (experimentally or numerically via MC simulations) directly by detecting the total received intensity in the considered detector [21]. Then, by varying μ_s (experimentally or numerically), $\partial \ln(P_R)/\partial \mu_s$ can be determined. The experimental evaluation of $\partial \ln(P_R)/\partial \mu_s$ is possible, e.g., for liquid scattering media, where a measurable increment of the scattering properties of the medium can be determined. The corresponding numerical evaluation in MC simulations is a trivial procedure.

Interestingly, the reliability of MC codes can also be tested by comparing the difference $\langle k\rangle_R/\mu_s - \langle \ell\rangle_R$, obtained by MC, against the same difference obtained from exact RTE solutions for P_R.

It is also maybe useful to note that, the formal expressions for the TD (Eq. (4)), and for the CW domain (Eq. (5)), are the starting points for the scaling formulas used in MC simulators applied to describe variations of the absorption and scattering coefficients over the whole medium. Consequently, the obtained relations are also at the basis of the so-called perturbation and differential Monte Carlo methods [23,35–42]. Expressions for the “Adding absorption” and “Adding scattering” were reported in the previous literature for the TD [23], while a CW counterpart was missing.

From an experimental standpoint, the “Adding scattering” protocol is particularly convenient in calibrated liquid phantoms. Intralipid 20 % is widely used as a reference scattering medium and its optical properties have been extensively characterized [43,44]. Controlled dilutions therefore provide accurate and reproducible increments of μ_s (with minimal concomitant change in μ_a at suitable wavelengths), enabling a direct experimental implementation of finite-difference estimates of $\partial \ln(P_R)/\partial \mu_s$. In Section 3.4 we report such a measurement, which serves as an experimental validation of the “Adding scattering” method and of the associated identities.

3. Applications and validation on the obtained relations

In this section, we illustrate how the exact identities derived above can be used in practice. We first present two conceptual applications: (i) relations between mean fluence, mean pathlength, and mean number of scatterings (Section 3.1); and (ii) a reformulation of the invariance property in terms of $\langle k\rangle/\mu_s$ (Section 3.2). We then provide numerical validation using independent Monte Carlo implementations (Section 3.3), highlighting how the identities can serve as exact benchmarks for forward solvers. Finally, we demonstrate the “Adding scattering” method experimentally in calibrated liquid phantoms (Section 3.4).

3.1. Relationships for mean fluence, mean pathlength and mean number of scattering events

The relationships obtained in Subsection 2.3, linking the absorbed power to the mean pathlength and to the mean number of scattering events, can be also used to obtain relationships for the mean fluence rate, a significant radiometric quantity widely used in radiative transfer [6,8,45].

Denoting with $\Phi(\boldsymbol{r})$ the fluence rate at $\boldsymbol{r}$, and recalling that the product $\mu_a\Phi(\boldsymbol{r})\mathrm{d}\boldsymbol{r}$ represents the fraction of power absorbed in the volume element $\mathrm{d}\boldsymbol{r}$, the fraction of absorbed power in V_i with absorption coefficient $\mu_{a,i}$ can be expressed as:

$$\frac{P^{T}_{A_i^*}}{P_E} = \mu_{a,i}\int_{V_i}\frac{\Phi(\boldsymbol{r})}{P_E}\mathrm{d}\boldsymbol{r} = \mu_{a,i}\frac{\langle\Phi\rangle^{T}_{E,i}}{P_E}V_i, \tag{55}$$

where $\langle\Phi\rangle^{T}_{E,i}$ is the mean fluence in V_i, usually denoted in literature simply as $\langle\Phi\rangle_{V_i}$.

From Eqs. (46) and (55) we obtain an exact relationship between the mean fluence and the mean pathlength:

$$\frac{\langle\Phi\rangle^{T}_{E,i}}{P_E} = \frac{\langle\ell_i\rangle^{T}_{E}}{V_i}, \tag{56}$$

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and from Eqs. (49) and (56) an exact relationship between the mean fluence and the mean number of scattering events:

$$\frac{\langle \Phi \rangle_{\mathrm{E},i}^{\mathrm{T}}}{P_{\mathrm{E}}} = \frac{1}{\mu_{\mathrm{s},i}} \frac{\langle k \rangle_{\mathrm{E},i}^{\mathrm{T}}}{V_i}. \tag{57}$$

The relationship between the mean fluence and the mean pathlength (Eq. (56)) is intrinsic to the definition of fluence, see for instance the works devoted to dosimetry in nuclear physics [46–49], which have been also recently demonstrated following a radiative transfer approach [45]. On the other hand, to the best of our knowledge, the exact relationship between mean fluence and mean number of scattering events in the form of Eq. (57) has not been previously presented in photon migration studies.

It is worth noting that, in the present contribution Eq. (56) arises from very basic principles of light scattering and absorption, while the previous proof shown in [45] was based on a quite complex procedure using the concept of generalized fluence rate.

3.2. *Invariance property for ratio between number of scattering events and scattering coefficient*

It is well known from the literature that the "invariance property" (IP) expresses the total mean pathlength $\langle \ell \rangle_{\mathrm{E}}^{\mathrm{T}}$ spent by photons inside a finite *non-absorbing* homogeneous volume V — when externally illuminated with a uniform and isotropic radiance (Lambertian illumination) [17,18] — as

$$\langle \ell \rangle_{\mathrm{E}}^{\mathrm{T}} = 4 \left(\frac{n}{n_e} \right)^2 \frac{V}{S}, \tag{58}$$

where S, n and n_e are the V surface, the internal refractive index and, the external refractive index, respectively. By exploiting the results obtained in the present contribution, we will revisit the IP and gain new insight on this fundamental property.

By substituting Eq. (24) into Eq. (58), with the only restriction to have $\mu_{\mathrm{s}} \neq 0$ if $n > n_e$, one obtains

$$\frac{\langle k \rangle_{\mathrm{E}}^{\mathrm{T}}}{\mu_{\mathrm{s}}} = 4 \left(\frac{n}{n_e} \right)^2 \frac{V}{S}, \tag{59}$$

showing that the IP can also be expressed through the ratio between the number of scattering events and the scattering coefficient. This information can help visualize the propagation of a photon packet: once the scattering coefficient in the medium is fixed, then $\langle k \rangle_{\mathrm{E}}^{\mathrm{T}}$ *is exactly determined by the geometry*.

Similarly, for a non-homogeneous medium with the condition $\mu_{\mathrm{a},i} = 0, \forall i \in \{1, 2, \ldots, M\}$, the IP can be expressed (see Eq. (1.51) in [17]) as

$$\langle \ell_i \rangle_{\mathrm{E}}^{\mathrm{T}} = 4 \left(\frac{n_i}{n_e} \right)^2 \frac{V_i}{S}, \tag{60}$$

where V_i is a (homogeneous) sub-volume of V, S the surface of V and, n_i the refractive index of V_i. By inserting Eq. (48) in Eq. (60), we obtain

$$\frac{\langle k \rangle_{\mathrm{E},i}^{\mathrm{T}}}{\mu_{\mathrm{s},i}} = 4 \left(\frac{n_i}{n_e} \right)^2 \frac{V_i}{S}. \tag{61}$$

The IP for the ratio between the average number of scattering events and the scattering coefficient is therefore also valid for the non-homogeneous medium.

3.3. Monte Carlo validation

In this subsection, we show how the identities derived in Subsection 2.6 can be used as stringent internal consistency checks (and thus benchmarks) for Monte Carlo photon transport solvers. In particular, for any chosen sub-volume V_i the absorbed-power fraction $P^{\mathrm{T}}_{\mathrm{A}_i^*}/P_{\mathrm{E}}$ must satisfy both Eqs. (46) and (49), i.e., it can be expressed equivalently in terms of (i) the mean pathlength $\langle \ell_i \rangle^{\mathrm{T}}_{\mathrm{E}}$ spent in V_i by all emitted photons and (ii) the mean number of scattering events $\langle k \rangle^{\mathrm{T}}_{\mathrm{E},i}$ occurring in V_i. Because these quantities can be tallied in MC simulations using different estimators, their exact equivalence provides a sensitive way to detect subtle implementation biases.

To illustrate this use, we performed simulations with two independent estimators: the albedo weight (AW) and microscopic Beer–Lambert–Bouguer (mBLB) methods [50] both implemented with Russian roulette for packet termination; without Russian roulette, $\epsilon_{\langle \ell_i \rangle}$ (for mBLB) or $\epsilon_{\langle k \rangle_i}$ (for AW) would vanish identically by construction. For each layer V_i, we computed $P^{\mathrm{T}}_{\mathrm{A}_i^*}/P_{\mathrm{E}}$, $\langle \ell_i \rangle^{\mathrm{T}}_{\mathrm{E}}$, and $\langle k \rangle^{\mathrm{T}}_{\mathrm{E},i}$, and we quantified the residuals of Eqs. (46) and (49) through the following normalized statistics:

$$\epsilon_{\langle \ell_i \rangle} = \frac{P^{\mathrm{T}}_{\mathrm{A}_i^*}/P_{\mathrm{E}} - \mu_{\mathrm{a},i} \langle \ell_i \rangle^{\mathrm{T}}_{\mathrm{E}}}{\mathrm{SE}\left(P^{\mathrm{T}}_{\mathrm{A}_i^*}/P_{\mathrm{E}} - \mu_{\mathrm{a},i} \langle \ell_i \rangle^{\mathrm{T}}_{\mathrm{E}} \right)}, \quad \epsilon_{\langle k \rangle_i} = \frac{P^{\mathrm{T}}_{\mathrm{A}_i^*}/P_{\mathrm{E}} - \mu_{\mathrm{a},i} \frac{\langle k \rangle^{\mathrm{T}}_{\mathrm{E},i}}{\mu_{\mathrm{s},i}}}{\mathrm{SE}\left(P^{\mathrm{T}}_{\mathrm{A}_i^*}/P_{\mathrm{E}} - \mu_{\mathrm{a},i} \frac{\langle k \rangle^{\mathrm{T}}_{\mathrm{E},i}}{\mu_{\mathrm{s},i}} \right)}. \tag{62}$$

Here SE(·) denotes the statistical standard error of the numerator. If the identities are satisfied within statistical uncertainty, $\epsilon_{\langle \ell_i \rangle}$ and $\epsilon_{\langle k \rangle_i}$ should fluctuate around zero; practically, values within about one standard error (i.e. in $(-1, 1)$) indicate agreement at the expected statistical level.

Simulations were carried out for a homogeneous slab with thickness 20 mm, divided into 10 layers of 2 mm, with refractive index 1.4 and reduced scattering coefficient $\mu_s' = 1\,\mathrm{mm}^{-1}$; the external refractive index was 1. For each layer, the MC tallies return $P^{\mathrm{T}}_{\mathrm{A}_i^*}/P_{\mathrm{E}}$, $\langle \ell_i \rangle^{\mathrm{T}}_{\mathrm{E}}$, and $\langle k \rangle^{\mathrm{T}}_{\mathrm{E},i}$ from which $\epsilon_{\langle \ell_i \rangle}$ and $\epsilon_{\langle k \rangle_i}$ are computed. Details on the MC code employed can be found in [8].

Figure 5 reports $\epsilon_{\langle \ell_i \rangle}$ and $\epsilon_{\langle k \rangle_i}$ versus depth for $\mu_a = 0.1\,\mathrm{mm}^{-1}$. Results were obtained by simulating 10^8 trajectories for both isotropic and anisotropic scattering and each quantity calculated from the simulation is finally expressed by its mean value with its associated standard error. For completeness, we note that in the absence of Russian roulette the residuals $\epsilon_{\langle \ell_i \rangle}$ (for mBLB) and $\epsilon_{\langle k \rangle_i}$ (for AW) vanish identically by construction, so that in these specific cases the benchmark is expected to be perfectly satisfied and does not carry statistical significance. In all other cases, for all layers and for both independent MC implementations (AW and mBLB, with and without Russian roulette), the normalized residuals remain largely within one standard error, confirming the identities at the level set by Monte Carlo statistics. This example illustrates how Eqs. (46) and (49) can serve as exact, implementation-independent benchmarks to validate MC solvers and to detect small systematic inconsistencies in tallies of absorbed power, pathlength, or collision number.

3.4. Experimental validation of the “adding scattering” method

Measurements were performed on samples of Intralipid 20 % diluted in purified water housed inside a cylindrical container of dimensions simulating an infinite homogeneous medium and thus much larger than the source-detector distances considered in the experiments. An illustrative picture of the experimental configuration is shown in Fig. 6(a), with more details on the setup available in previous publications [21,43]. Two identical plastic fibers terminated by 0.5 mm-diameter diffusing tips were used for illumination (using a 3 mW diode laser) and collection (using a photomultiplier and a lock-in amplifier). The center-to-center source–detector distance r was varied by a computer-controlled translation stage between $10 \le r \le 34$ mm in 1 mm steps. The error on the relative displacement was (0.002 mm), however the uncertainty in positioning

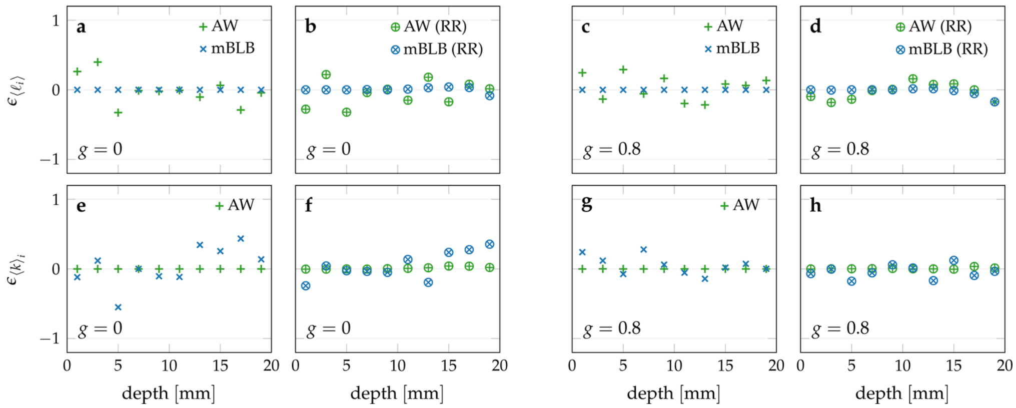

Fig. 5. Equivalence between the different methods for computing the fluence (Albedo Weight and microscopic Beer–Lambert–Bouguer, without and with Russian roulette). Simulations are performed for a 20 mm-thick homogeneous scattering slab subdivided into 10 layers. The slab has a refractive index of 1.4, $\mu_s' = 1\,\mathrm{mm}^{-1}$ and $\mu_a = 0.1\,\mathrm{mm}^{-1}$. Panels are grouped by scattering anisotropy ($g = 0$ or $g = 0.8$) and by the use of a Russian roulette (RR) method. In the case without RR, $\epsilon_{\langle \ell_i \rangle}$ and $\epsilon_{\langle k \rangle_i}$ are expected to vanish by construction for the mBLB and AW cases, respectively, as confirmed by the numerical result.

the fibers can lead to a overall uncertainty of 0.1 mm on r. The received power P_R for all the distances was measured for different concentration of Intralipid 20 %, i.e., different values of the scattering coefficient of the medium. A wavelength 751 nm was chosen because the absorption coefficients of water and Intralipid are nearly identical at this wavelength, so that changing the Intralipid concentration produces a change in scattering while leaving absorption essentially unchanged.

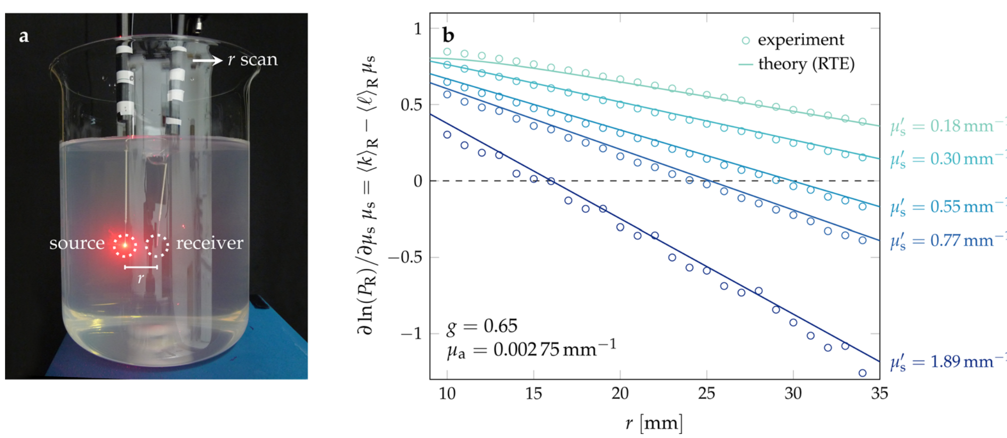

Fig. 6. (a) Scattering cell filled with diluted Intralipid and source/receiving fibers. (b) Values of $\langle k \rangle_R - \langle \ell \rangle_R \mu_s$ obtained from measurements (markers, inferred from the measured dependence $P_R(\mu_s)$ through Eq. (63)) and from an exact RTE prediction (solid lines, obtained by differentiating the RTE prediction for $P_R(\mu_s)$) versus the source–detector distance r. In the RTE calculation, the absorption coefficient was set to that of water at 751 nm, while the phase-function asymmetry factor g was taken from [43,51] and a HG model was assumed.

Figure 6(b) reports the quantity $\langle k \rangle_R - \langle \ell \rangle_R \mu_s$ as obtained both experimentally and numerically versus the source-receiver distance r for different values of the scattering coefficient of the medium. The evaluation follows the exact chain of identities

$$\frac{\partial \ln(P_\mathrm{R})}{\partial \mu_\mathrm{s}}\mu_\mathrm{s} = \langle k\rangle_\mathrm{R} - \langle \ell\rangle_\mathrm{R}\mu_\mathrm{s} = \frac{\partial \ln(P_\mathrm{R})}{\partial \mu_\mathrm{s}'}\mu_\mathrm{s}', \tag{63}$$

with $\mu_\mathrm{s}' = \mu_\mathrm{s}(1-g)$ the reduced scattering coefficient. Experimentally, $\partial \ln(P_\mathrm{R})/\partial \mu_\mathrm{S}$ (or equivalently $\partial \ln(P_\mathrm{R})/\partial \mu_\mathrm{s}'$) was obtained by small finite differences around the targeted value. Therefore, the quantity plotted in Fig. 6(b) is the value inferred from the measured dependence $P_\mathrm{R}(\mu_\mathrm{s})$ through the exact identity of Eq. (63). The same finite-difference procedure was applied to the theoretical $P_\mathrm{R}(\mu_\mathrm{s})$ curves, so that the comparison in Fig. 6(b) is performed under the same operational definition in both experiment and theory. The curves shown in Fig. 6(b) correspond to different scattering conditions spanning more than one order of magnitude in reduced scattering strength, demonstrating that the discrepancy is measurable across a broad range of transport regimes relevant to tissue optics. The Intralipid 20 % used in this study was from the same batch as a previously calibrated one [44], allowing μ_s (or μ_s') to be determined from concentration using the published calibration. Theoretical curves were computed using an exact solution of the RTE for an infinite homogeneous medium [52]. The agreement between measurements and theory is excellent over the explored distances and scattering values, and the quantity $\langle k\rangle_\mathrm{R} - \langle \ell\rangle_\mathrm{R}\mu_\mathrm{s}$ remains of order unity (in units of scattering events), i.e. it is small but clearly resolvable.

Two points are worth emphasizing. First, because Eq. (63) is based on a logarithmic derivative, the result is independent of absolute power calibration and of the units used for P_R, which makes the estimate particularly robust. Second, the measurements confirm that the mismatch $\langle k\rangle_\mathrm{R}/\mu_\mathrm{s} - \langle \ell\rangle_\mathrm{R}$ is not exactly zero. Although the approximation $\langle k\rangle_\mathrm{R} \approx \mu_\mathrm{s}\langle \ell\rangle_\mathrm{R}$ is often used as a useful heuristic in the diffusive regime, so that it is usually taken as an exact property, Eq. (9) shows that an exact equality would imply $\partial \ln(P_\mathrm{R})/\partial \mu_\mathrm{s} = 0$, i.e. vanishing sensitivity of the detected signal to scattering. The observed systematic (and sign-changing) deviation therefore has a direct physical interpretation in terms of scattering sensitivity and provides an experimentally accessible benchmark in photon migration studies.

4. Conclusion

In summary, the obtained relations for the homogeneous medium (Eqs. (22), (24) and (25)) are:

$$\frac{P_\mathrm{A}^\mathrm{T}}{P_\mathrm{E}} = \mu_\mathrm{a}\langle \ell\rangle_\mathrm{E}^\mathrm{T}, \qquad \frac{\langle k\rangle_\mathrm{E}^\mathrm{T}}{\mu_\mathrm{s}} = \langle \ell\rangle_\mathrm{E}^\mathrm{T}, \qquad \frac{P_\mathrm{A}^\mathrm{T}}{P_\mathrm{E}} = \frac{\mu_\mathrm{a}}{\mu_\mathrm{s}}\langle k\rangle_\mathrm{E}^\mathrm{T},$$

while those derived for the heterogeneous medium (Eqs. (46), (48) and (49)) are:

$$\frac{P_{\mathrm{A}_i^*}^\mathrm{T}}{P_\mathrm{E}} = \mu_{\mathrm{a},i}\langle \ell_i\rangle_\mathrm{E}^\mathrm{T}, \qquad \frac{\langle k\rangle_{\mathrm{E},i}^\mathrm{T}}{\mu_{\mathrm{s},i}} = \langle \ell_i\rangle_\mathrm{E}^\mathrm{T}, \qquad \frac{P_{\mathrm{A}_i^*}^\mathrm{T}}{P_\mathrm{E}} = \frac{\mu_{\mathrm{a},i}}{\mu_{\mathrm{s},i}}\langle k\rangle_{\mathrm{E},i}^\mathrm{T}.$$

These equations constitute two sets of exact identities that follow directly from the statistical interpretation of absorption and scattering in radiative transfer, and therefore hold without approximation for arbitrary geometries, source configurations, and detector arrangements, which is not easy to find in other existing solutions of the RTE. To our knowledge, only a limited number of relations with comparable scope, exactness and simplicity are known in photon migration, such as those related to the invariance property for the mean optical pathlength, or the statistics of scattering events in infinite media [17,53,54].

The findings presented here — though derived from radiative transfer theory — can be applied to other areas of transport theory, for physical phenomena that follow the same mathematical structure as the radiative transfer equation. This occurs when absorption coefficients and scattering properties can be clearly defined, allowing for interactions such as absorption and elastic scattering of the transported particles. Transport theory generally deals with the movement of particles through a background medium and is used in various applications where the particles and the medium they travel through may differ significantly in nature. Despite these differences, the underlying equations share a common form, reflecting fundamental principles like energy balance and the physical interpretation of absorption and scattering. As a result, diverse phenomena — whether involving neutrons, gas molecules, plasma atoms, electrons, photons, or other quantities — can all be described using similar core equations. Exploring how the derived relationships from this work can be adapted for other transport processes beyond radiative transfer would be valuable.

Fundamentally, this theory provides a simple yet essential representation of photon propagation in absorbing and scattering media using fundamental quantities from photon transport theory. Furthermore, as it is the case for the IP and for the statistics of scattering points in the infinite medium [17,53,54], the present results can also serve as benchmarks for verifying MC codes. For example, the relation $P^{\mathrm{T}}_{\mathrm{A}_i^*}/P_{\mathrm{E}} = \mu_{\mathrm{a},i}\langle \ell_i \rangle^{\mathrm{T}}_{\mathrm{E}}$ introduces a non-trivial validation test linked to key simulation parameters.

As shown in Table 1, the equivalence between $P^{\mathrm{T}}_{\mathrm{A}_i^*}/P_{\mathrm{E}}$, $\langle \ell_i \rangle^{\mathrm{T}}_{\mathrm{E}}$, $\langle k \rangle^{\mathrm{T}}_{E,i}$ and $\langle \Phi \rangle^{\mathrm{T}}_{\mathrm{E},i}$ enables the selection of three interchangeable MC methods for calculating $P^{\mathrm{T}}_{\mathrm{A}_i^*}/P_{\mathrm{E}}$ or $\langle \Phi \rangle^{\mathrm{T}}_{\mathrm{E},i}$, both of which are quantities of practical interest in many applications.

Table 1. Summary of the three MC methods allowing to assess $P^{\mathrm{T}}_{\mathrm{A}_i^*}/P_{\mathrm{E}}$ and $\langle \Phi \rangle^{\mathrm{T}}_{\mathrm{E},i}$; where $\mu_{\mathrm{a},i}$, $\mu_{\mathrm{s},i}$, V_i and P_{E} are the commonly known parameters of the MC simulation.

From MC calculation →	$P^{\mathrm{T}}_{\mathrm{A}_i^*}/P_{\mathrm{E}}$	$\langle \ell_i \rangle^{\mathrm{T}}_{\mathrm{E}}$	$\langle k \rangle^{\mathrm{T}}_{\mathrm{E},i}$
$P^{\mathrm{T}}_{\mathrm{A}_i^*}/P_{\mathrm{E}}$	$P^{\mathrm{T}}_{\mathrm{A}_i^*}/P_{\mathrm{E}}$	Eq. (46)	Eq. (49)
$\langle \Phi \rangle^{\mathrm{T}}_{\mathrm{E},i}$	Eq. (55)	Eq. (56)	Eq. (57)

In existing MC codes for biomedical optics applications, the photon fluence rate has primarily been calculated as a fraction of the total power absorbed in V_i. Recently, however, it has been proposed to compute fluence using Eq. (56) [45]. Conversely, Eq. (57) is currently not exploited, and its rigorous validity is demonstrated here for the first time. It is finally worth to note that results of Fig. 5 confirms, as expected from the obtained relations, that the three different ways to calculate the average photon fluence of Table 1 are equivalent.

These findings introduce additional and innovative computational options beyond those currently implemented in many open-source codes. These advancements could significantly impact the development of new MC codes in application fields such as tissue optics. The relations summarized in Table 1 have found a significant validation by MC simulations with the results of Fig. 5.

Besides providing a unified derivation of exact power–pathlength–collision identities for both homogeneous and heterogeneous media, this work highlights a consequence that is directly tied to scattering sensitivity. For received photons, Eq. (9) shows that the quantity $\langle k \rangle_{\mathrm{R}}/\mu_{\mathrm{s}} - \langle \ell \rangle_{\mathrm{R}}$ is not merely a small correction: it corresponds to the local scattering sensitivity of the detected signal.

From a practical viewpoint, the derived identities offer exact, implementation-independent benchmarks for MC and other forward solvers. In Section 3.3 we validated Eqs. (46) and (49) using independent MC estimators (AW and mBLB), finding agreement within statistical uncertainty across all layers, illustrating how these relations can detect subtle systematic biases in tallies of absorbed power, pathlength, or collision number. In Section 3.4 we further demonstrated that the same scattering-sensitivity identity can be probed experimentally through finite differences in μ_{s}, finding good agreement with an exact RTE prediction in the infinite-medium geometry.

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Although the mismatch is small (order unity in scattering events), it is systematic and measurable. Moreover, it can change sign with source–detector separation, implying the existence of a distance at which scattering sensitivity is locally minimized.

This counter-intuitive result can be used to design measurement geometries with controlled sensitivity to μ_s and to build refined tests for photon-transport solvers, besides deepening our general understanding of photon migration to go beyond a limited intuitive/heuristic view of the problem.

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