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# Interpretation of the failure of the time-independent diffusion equation near a point source

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**Abstract**

The time-independent diffusion equation (DE) yields inaccurate solutions near sources. To investigate this issue we solve a forward problem of light propagation from a time-independent isotropic point source in an infinite medium of constant refractive index, constant absorption coefficient and constant reduced scattering coefficient using the standard radiative transfer equation (RTE) and three recently reported RTEs. Only one of those equations yields solutions consistent with the results of Monte Carlo simulations in near field, due to its ability to model ray divergence. From that equation we derive a condition for neglecting the divergence of rays emitted by a point source in forward problems that is the same as the reported condition for the accuracy of the time-independent DE. These results strongly suggest that the inaccuracy of the time-independent DE near sources is due to a missing term describing ray divergence, a drawback inherited from the RTE. One of the studied RTEs and the derived equations are free of that drawback.


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## 1. Introduction

The diffusion equation (DE) is widely used for describing light propagation in biological tissues. However, it yields inaccurate solutions in the vicinity of sources. This issue has been studied by Fantini et al. [1],

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Kienle and Patterson [2], Rinzema et al. [3], Martelli et al. [4] and Graaff and Rinzema [5] among others. That drawback of the DE is important in practical situations, when it is of interest to calculate the dose of light applied or to retrieve the optical properties of the tissue near the light source. One of the factors affecting the accuracy of the DE in the vicinity of a source is the small quantity of scattering events undergone in that region by photons just emitted by it [3]. It should be noted also that the optical model on which the radiative transfer equation (RTE) and the DE are based assumes that the divergence of the rays is zero everywhere in the scattering medium [6]. However, this assumption is not valid near a source, where the ray divergence cannot be neglected [7]. It is another possible cause for the inaccuracy of the DE near sources.

In 1999 Ferwerda proposed a radiative transfer equation for media with spatially varying refractive index (RTEvri) [8]. Khan and Jiang [9] eliminated a redundant term of the Ferwerda RTEvri and derived a diffusion equation for media with spatially varying refractive index (DEvri). The Ferwerda–Khan–Jiang RTEvri accounts for spatial variations of refractive index and its effect on ray divergence. However, the Ferwerda model considers that the ray divergence depends on the gradient of logarithm of refractive index and, consequently, yields zero ray divergence in media with constant refractive index. Tualle and Tinet derived another RTEvri [10]. The physical model leading to the Tualle-Tinet RTEvri assumes that the ray divergence is zero everywhere. Consequently, it cannot describe the effects related to spatial variations of the ray divergence. In a recent paper Martí-López et al. modified the divergence term of the Ferwerda–Khan–Jiang RTEvri and obtained the Martí–Bouza–Hebden–Arridge–Martínez RTEvri [7]. Although all those equations were derived to account for spatial variation of refractive index, they also present specific expressions for the ray divergence due to the use of different ray models. Obviously they must be carefully compared to determine which ray model provides a better description of light propagation. This comparison can be accomplished by solving problems of light propagation in turbid medium with well-known solutions.

The problem of propagation of an optical field emitted by a time-independent isotropic point source in an infinite medium of constant refractive index, constant absorption coefficient and constant reduced scattering coefficient (uniform infinite medium) has been extensively studied both theoretically [6,4] and experimentally [3,4]. In addition isotropic point sources in an uniform medium have been simulated by Monte Carlo methods [4,11] and the divergence of rays emerging from a point source can be easily calculated [7]. These circumstances encourage the use of that problem as a benchmark for testing above equations.

The ultimate goal of this paper is to compare the RTE, the Ferwerda–Khan–Jiang RTEvri, the Tualle–Tinet RTEvri, the Martí–Bouza–Hebden–Arridge–Martínez RTEvri and Monte Carlo simulations in the solution of the problem of propagation of an optical field emitted by a time-independent isotropic point source in an uniform infinite medium. First we discuss in detail the physical model leading to the Martí–Bouza–Hebden–Arridge–Martínez RTEvri and derive a new DEvri, a new diffusion coefficient, a RTE for media with constant refractive index and rays of arbitrary divergence (RTErad) and a DE for media with constant refractive index and rays of arbitrary divergence (DErad). Afterwards we analyze an isotropic point source in uniform infinite medium and obtain two sets of differential equations for this problem. The first one is composed of the $P_1$ approximation of the RTErad and the derived DErad. The second one is composed of the $P_1$ approximation of the standard RTE and the corresponding DE. The latter set of equations can be obtained from the first one on the condition of zero ray divergence. We show that the Ferwerda–Khan–Jiang RTEvri and Tualle–Tinet RTEvri reduce to the standard RTE in this specific case. To find approximate solutions to the first set of equations we introduce a critical radius $R_{\mathrm{crit}}$, which defines three propagation zones, namely, near field ($r \ll R_{\mathrm{crit}}$), middle field ($r \sim R_{\mathrm{crit}}$) and far field ($r \gg R_{\mathrm{crit}}$), where $r$ is the distance to the point source. We obtain the near-field and the far-field solutions to the DErad for the time-independent isotropic point source in uniform medium. The far-field solutions to the DErad are also solutions to the standard DE. Those solutions are compared with Monte Carlo simulations for four sets of parameters of the medium. The near-field solutions and the far-field solutions agree well with Monte Carlo results in their corresponding zones. We note that the far-field condition $r \gg R_{\mathrm{crit}}$ coincides with the condition for the accuracy of the DE derived by Rinzema et al. [3] for forward tasks and derive the radius of the region of inaccuracy of the standard DE for inverse tasks. Finally, we analyze our results and conclude that the good agreement of the near-field solutions and the far-field solutions with Monte Carlo results in their corresponding zones of validity and the equivalence of the far-field condition and the condition for the accuracy of DE suggest that the failure of the DE near a point source is due to the absence or the inadequate form of a term describing the ray divergence in the RTE, the Ferwerda–Khan–Jiang RTEvri and the Tualle–Tinet RTEvri, a drawback that the Martí–Bouza–Hebden–Arridge–Martínez RTEvri does not present.

## 2. The diffusion equation for media with spatially varying refractive index

### 2.1. Physical model

The model leading to the Martí–Bouza–Hebden–Arridge–Martínez RTEvri can be described as a two stage model. At the first stage it is considered that wave fronts and rays of non-polarized light propagate in a background medium with refractive index $n(\mathbf{r})$, being $\mathbf{r}$ the coordinate of a point of the medium. The wave fronts are described by eikonals $\Lambda(\mathbf{r})$, given by the equation [13]:

$$\nabla_{\mathbf{r}}\Lambda(\mathbf{r}) \cdot \nabla_{\mathbf{r}}\Lambda(\mathbf{r}) = n^2(\mathbf{r}), \tag{1}$$

with adequate boundary conditions and wave front source distributions. Here symbol $\nabla_{\mathbf{r}}$ denotes the gradient operator:

$$\nabla_{\mathbf{r}} = \frac{\partial}{\partial x_1}\hat{\mathbf{x}}_1 + \frac{\partial}{\partial x_2}\hat{\mathbf{x}}_2 + \frac{\partial}{\partial x_3}\hat{\mathbf{x}}_3,$$

and $\hat{\mathbf{x}}_1,\ \hat{\mathbf{x}}_2,\ \hat{\mathbf{x}}_3$ are the unit vectors of the Cartesian coordinate system. A wave front surface is specified by the expression $\Lambda(\mathbf{r})$ = constant [13].

The equation of the trajectory of a ray $\mathbf{r} = \mathbf{R}(s)$, $s$ being the arc length, can be derived from Eq. (1) [13]

$$\frac{\mathrm{d}}{\mathrm{d}s}\left\{n[\mathbf{R}(s)]\frac{\mathrm{d}}{\mathrm{d}s}\mathbf{R}(s)\right\} = \nabla_{\mathbf{r}} n[\mathbf{R}(s)]. \tag{2}$$

The unit vector $\mathbf{\Omega}$, perpendicular to the wave front and tangent to the ray trajectory of the ray passing through the point $r$, can be calculated with the expressions:

$$\mathbf{\Omega}(\mathbf{r}) = \frac{\nabla_{\mathbf{r}}\Lambda(\mathbf{r})}{n(\mathbf{r})}, \tag{3}$$

$$\mathbf{\Omega}[\mathbf{r}(s)] = \frac{\mathrm{d}}{\mathrm{d}s}\mathbf{R}(s). \tag{4}$$

From Eqs. (2) and (4) it follows that [13]:

$$\frac{\mathrm{d}}{\mathrm{d}s}\{n[\mathbf{R}(s)]\mathbf{\Omega}[\mathbf{R}(s)]\} = \nabla_{\mathbf{r}} n[\mathbf{R}(s)]. \tag{5}$$

At a second stage the processes of absorption and scattering are introduced. We consider that the background medium absorbs light and that scattering centers are distributed in it. Nonlinear effects and inelastic scattering are neglected. Repeating the core idea of Professor Ferwerda, we write the energy balance in an elementary scattering volume $\Delta V$ embedded in a ray congruency as [8]:

$$L[\mathbf{r}+\Delta\mathbf{r},\boldsymbol{\Omega}(\mathbf{r}+\Delta\mathbf{r}),t+\Delta t]A' - L[\mathbf{r},\boldsymbol{\Omega}(\mathbf{r}),t]A = -[\mu_a(\mathbf{r})+\mu_s(\mathbf{r})]L(\mathbf{r},\boldsymbol{\Omega},t)\Delta V + \mu_s(\mathbf{r})\Delta V \times \int_{4\pi}\theta(\mathbf{r},\Omega,\Omega')L(\mathbf{r},\boldsymbol{\Omega}',t)\,\mathrm{d}\omega' + \epsilon(\mathbf{r},\boldsymbol{\Omega},t)\Delta V, \tag{6}$$

where $L(\mathbf{r},\boldsymbol{\Omega},t)$ is the radiance at a point $\mathbf{r}$ in the direction $\boldsymbol{\Omega}(\mathbf{r}) = \Omega_1\hat{\mathbf{x}}_1 + \Omega_2\hat{\mathbf{x}}_2 + \Omega_3\hat{\mathbf{x}}_3$, $\boldsymbol{\Omega}(\mathbf{r})$ is the unit vector perpendicular to the wave front or, equivalently tangent to the ray, $\Delta\mathbf{r}$ is the displacement of position, $\mu_a(\mathbf{r})$ and $\mu_s(\mathbf{r})$ are the absorption and scattering coefficients, respectively, $\Delta V \approx \Delta sA$ is the elementary scattering volume, $\theta(\mathbf{r},\boldsymbol{\Omega},\boldsymbol{\Omega}')$ is the normalized scattering function, $\boldsymbol{\Omega}'$ is the direction of propagation of an incident ray scattered into direction $\boldsymbol{\Omega}$, $\mathrm{d}\omega'$ is a differential of solid angle, $\epsilon(\mathbf{r},\boldsymbol{\Omega},t)$ is the distribution of sources. See Fig. 1.

Now we need to find the relations between $L(\mathbf{r}+\Delta\mathbf{r},\boldsymbol{\Omega}(\mathbf{r}+\Delta\mathbf{r}),t+\Delta t)$ and $L(\mathbf{r},\boldsymbol{\Omega}(\mathbf{r}),t)$ as well as between $A'$ and $A$. The expansion in Taylor's series of $L(\mathbf{r}+\Delta\mathbf{r},\boldsymbol{\Omega}(\mathbf{r}+\Delta\mathbf{r}),t+\Delta t)$ on the variables $\mathbf{r}$ and $t$ yields

$$\begin{aligned} L(\mathbf{r}+\Delta\mathbf{r},\boldsymbol{\Omega}(\mathbf{r}+\Delta\mathbf{r}),t+\Delta t) &= L(\mathbf{r},\boldsymbol{\Omega},t) + \frac{\partial}{\partial t}L(\mathbf{r},\boldsymbol{\Omega},t)\Delta t + \sum_{i=1}^{3}\frac{\partial L\left(\overset{\downarrow}{\mathbf{r}},\boldsymbol{\Omega},t\right)}{\partial x_i}\Delta x_i \\ &+ \sum_{i=1}^{3}\sum_{j=1}^{3}\left.\frac{\partial L(\mathbf{r},\boldsymbol{\Omega},t)}{\partial\Omega_j}\right|_{|\boldsymbol{\Omega}|=1}\left.\frac{\partial\Omega_j}{\partial x_i}\right|_{|\boldsymbol{\Omega}|=1}\Delta x_i = L(\mathbf{r},\boldsymbol{\Omega},t) + \frac{\partial}{\partial t}L(\mathbf{r},\boldsymbol{\Omega},t)\Delta t \\ &+ \nabla_{\mathbf{r}}L(\overset{\downarrow}{\mathbf{r}},\boldsymbol{\Omega},t)\cdot\Delta\mathbf{r} + \nabla_{\boldsymbol{\Omega}}L(\mathbf{r},\boldsymbol{\Omega},t)|_{|\boldsymbol{\Omega}|=1}\cdot\Delta\boldsymbol{\Omega}|_{|\boldsymbol{\Omega}|=1}, \end{aligned} \tag{7}$$

where $\Delta\boldsymbol{\Omega}|_{|\boldsymbol{\Omega}|=1} = \boldsymbol{\Omega}(\mathbf{r}+\Delta\mathbf{r}) - \boldsymbol{\Omega}(\mathbf{r})$ is the variation of direction of propagation:

$$\Delta\boldsymbol{\Omega}|_{|\boldsymbol{\Omega}|=1} = \left.\begin{pmatrix}\Delta\Omega_1\\ \Delta\Omega_2\\ \Delta\Omega_3\end{pmatrix}\right|_{|\boldsymbol{\Omega}|=1} = \left.\begin{pmatrix}\frac{\partial\Omega_1}{\partial x_1} & \frac{\partial\Omega_1}{\partial x_2} & \frac{\partial\Omega_1}{\partial x_3}\\ \frac{\partial\Omega_2}{\partial x_1} & \frac{\partial\Omega_2}{\partial x_2} & \frac{\partial\Omega_2}{\partial x_3}\\ \frac{\partial\Omega_3}{\partial x_1} & \frac{\partial\Omega_3}{\partial x_2} & \frac{\partial\Omega_3}{\partial x_3}\end{pmatrix}\right|_{|\boldsymbol{\Omega}|=1}\Delta\mathbf{r}. \tag{8}$$

Note that in expression (7) the operator $\nabla_{\mathbf{r}}$ does not act on the direction of propagation $\boldsymbol{\Omega}(\mathbf{r})$ of the radiance $L(\mathbf{r},\boldsymbol{\Omega}(\mathbf{r}),t)$ due to the use of vector $\boldsymbol{\Omega}(\mathbf{r})$ as an independent variable for the series expansion. This circumstance is important for further calculations. When the gradient operator does not act on the radiance $L(\mathbf{r},\boldsymbol{\Omega},t)$ it works as usually. Whenever a confusion could arise we use the arrow, as shown in expression (7) to mark the variable on which gradient operator acts. The operator $\nabla_{\boldsymbol{\Omega}}$ is defined as

$$\nabla_{\Omega}L(\mathbf{r},\boldsymbol{\Omega},t)|_{|\boldsymbol{\Omega}|=1} = \left.\frac{\partial L(\mathbf{r},\boldsymbol{\Omega},t)}{\partial\Omega_1}\right|_{|\boldsymbol{\Omega}|=1}\hat{\mathbf{x}}_1 + \left.\frac{\partial L(\mathbf{r},\boldsymbol{\Omega},t)}{\partial\Omega_2}\right|_{|\boldsymbol{\Omega}|=1}\hat{\mathbf{x}}_2 + \left.\frac{\partial L(\mathbf{r},\boldsymbol{\Omega},t)}{\partial\Omega_3}\right|_{|\boldsymbol{\Omega}|=1}\hat{\mathbf{x}}_3. \tag{9}$$

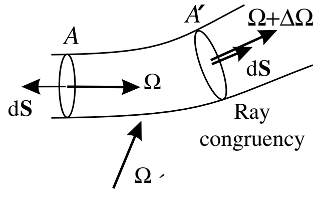


Fig. 1. Elementary scattering volume.

The radiance $L(\mathbf{r},\boldsymbol{\Omega},t)$ and the vector $\nabla_{\boldsymbol{\Omega}}L(\mathbf{r},\Omega,t)$ occurring in (7) require a particular analysis. The radiance $L(\mathbf{r},\boldsymbol{\Omega},t)$ is defined in two different spaces, the $\mathbf{r}$–$t$ space and the space of the unit normals to the wave fronts, or the unit tangents to ray trajectories, $\boldsymbol{\Omega}$ (the $\boldsymbol{\Omega}$ space). To find a simpler form of operator $\nabla_{\boldsymbol{\Omega}}$ we introduce the change of coordinates:

$$\Omega_1 = \sin\theta_\Omega \cos\varphi_\Omega, \quad \Omega_2 = \sin\theta_\Omega \sin\varphi_\Omega, \quad \Omega_3 = \cos\theta_\Omega, \quad 0 \leqslant \theta_\Omega < \pi,\ 0 \leqslant \varphi_\Omega < 2\pi, \tag{10}$$

which automatically satisfies the condition:

$$\Omega_1^2 + \Omega_2^2 + \Omega_3^2 = 1. \tag{11}$$

In this coordinate system the operator $\nabla_{\boldsymbol{\Omega}}$ has the form:

$$\nabla_{\hat{\theta}_\Omega \hat{\varphi}_\Omega} = \frac{\partial}{\partial\theta_\Omega}\hat{\boldsymbol{\theta}}_\Omega + \frac{1}{\sin\theta_\Omega}\frac{\partial}{\partial\varphi_\Omega}\hat{\varphi}_\Omega, \tag{12}$$

where $\hat{\boldsymbol{\theta}}_\Omega,\ \hat{\varphi}_\Omega$ are unit vectors. Note that vectors $\hat{\boldsymbol{\theta}}_\Omega$ and $\hat{\varphi}_\Omega$ are normal to vector $\boldsymbol{\Omega}$:

$$\hat{\theta}_\Omega \cdot \boldsymbol{\Omega} = \hat{\varphi}_\Omega \cdot \boldsymbol{\Omega} = 0. \tag{13}$$

This property was used by Khan and Jiang to eliminate a redundant term from the Ferwerda RTEvri [9].

The relation between $A'$ and $A$ can be found easily because the elementary scattering volume is embedded inside a ray congruency and no ray of that ray congruency can exit the volume through its lateral surface. Therefore, the flux of vector $\boldsymbol{\Omega}$ through the surface $\sigma$ of the elementary scattering volume $\Delta V$ is

$$\oint_\sigma \boldsymbol{\Omega}\,\mathrm{d}\mathbf{S} = A' - A, \tag{14}$$

where we assume that the surface is oriented outwards and $A' > 0$, $A > 0$.

Applying the Gauss theorem and the theorem of the mean value we obtain:

$$\oint_\sigma \boldsymbol{\Omega}(\mathbf{r})\,\mathrm{d}\mathbf{S} = \int_{\Delta V} \nabla_\mathbf{r}\cdot\boldsymbol{\Omega}(\mathbf{r})\,\mathrm{d}V \Rightarrow A' - A = \nabla_\mathbf{r}\cdot\boldsymbol{\Omega}(\mathbf{r})\Delta V \Rightarrow A' = \nabla_\mathbf{r}\cdot\boldsymbol{\Omega}(\mathbf{r})\Delta V + A, \tag{15}$$

where $\mathbf{r} \in \Delta V$. Note that in expression (15) the operator $\nabla_\mathbf{r}$ acts on the variable of the direction of propagation $\Omega$. Substituting expressions (7) and (15) in the expression (6) and using the relations

$$\Delta t = \frac{n(\mathbf{r})}{c}\Delta s, \quad \Delta\mathbf{r} = \boldsymbol{\Omega}(\mathbf{r})\Delta s, \tag{16}$$

we obtain:

$$\begin{aligned}
&\frac{n(\mathbf{r})}{c}\frac{\partial}{\partial t}L(\mathbf{r},\boldsymbol{\Omega},t) + \boldsymbol{\Omega}\cdot\nabla_\mathbf{r}L(\mathbf{r},\boldsymbol{\Omega},t) + [\nabla_\mathbf{r}\cdot\boldsymbol{\Omega}(\mathbf{r})]L(\mathbf{r},\boldsymbol{\Omega},t) + \nabla_{\boldsymbol{\Omega}}L(\mathbf{r},\boldsymbol{\Omega},t)\cdot\frac{\Delta\boldsymbol{\Omega}}{\Delta s} + [\nabla_\mathbf{r}\cdot\boldsymbol{\Omega}(\mathbf{r})]\frac{n(\mathbf{r})}{c}\\
&\quad\times\frac{\partial}{\partial t}L(\mathbf{r},\boldsymbol{\Omega},t)\Delta s + [\nabla_\mathbf{r}\cdot\boldsymbol{\Omega}(\mathbf{r})]\boldsymbol{\Omega}\cdot\nabla_\mathbf{r}L(\mathbf{r},\boldsymbol{\Omega},t)\Delta s + [\nabla_\mathbf{r}\cdot\boldsymbol{\Omega}(\mathbf{r})]\nabla_{\boldsymbol{\Omega}}L(\mathbf{r},\boldsymbol{\Omega},t)\cdot\frac{\Delta\boldsymbol{\Omega}}{\Delta s}\Delta s\\
&\qquad = -[\mu_\mathrm{a}(\mathbf{r}) + \mu_\mathrm{s}(\mathbf{r})]L(\mathbf{r},\boldsymbol{\Omega},t) + \mu_\mathrm{s}(\mathbf{r})\int_{4\pi}\theta(\mathbf{r},\boldsymbol{\Omega},\boldsymbol{\Omega}')L(\mathbf{r},\boldsymbol{\Omega}',t)\,\mathrm{d}\omega' + \epsilon(\mathbf{r},\boldsymbol{\Omega},t).
\end{aligned} \tag{17}$$

In the expression (17) the element of volume $\Delta V$ was cancelled out. Taking the limit $\Delta V = A\Delta s \to 0$ we obtain

$$\begin{aligned}
&\frac{n(\mathbf{r})}{c}\frac{\partial}{\partial t}L(\mathbf{r},\boldsymbol{\Omega},t) + \boldsymbol{\Omega}\cdot\nabla_\mathbf{r}L(\mathbf{r},\boldsymbol{\Omega},t) + [\nabla_\mathbf{r}\cdot\boldsymbol{\Omega}(\mathbf{r})]L(\mathbf{r},\boldsymbol{\Omega},t) + \nabla_{\boldsymbol{\Omega}}L(\mathbf{r},\boldsymbol{\Omega},t)\cdot\frac{\mathrm{d}\boldsymbol{\Omega}}{\mathrm{d}s}\\
&\quad = -[\mu_\mathrm{a}(\mathbf{r}) + \mu_\mathrm{s}(\mathbf{r})]L(\mathbf{r},\boldsymbol{\Omega},t) + \mu_\mathrm{s}(\mathbf{r})\int_{4\pi}\theta(\mathbf{r},\boldsymbol{\Omega},\boldsymbol{\Omega}')L(\mathbf{r},\boldsymbol{\Omega}',t)\,\mathrm{d}\omega' + \epsilon(\mathbf{r},\boldsymbol{\Omega},t).
\end{aligned} \tag{18}$$

This is the basic RTEvri [8]. Now we analyze the terms $\nabla_{\mathbf{r}} \cdot \mathbf{\Omega}(\mathbf{r})$, $d\mathbf{\Omega}/ds$ and $\theta(\mathbf{r},\mathbf{\Omega},\mathbf{\Omega}')$ occurring in expression (18).

### 2.2. The term $\nabla_{\mathbf{r}} \cdot \mathbf{\Omega}(\mathbf{r})$

In the common formulation of the radiative transfer theory the divergence term is assumed to be zero [6]. Tualle and Tinet assume also a zero ray divergence [10]. Obviously, this assumption does not allow modeling of the effect of a spatially varying refractive index on ray divergence. The divergence term $\nabla_{\mathbf{r}} \cdot \mathbf{\Omega}(\mathbf{r})$ was proposed to be [8]:

$$\begin{aligned}\nabla_{\mathbf{r}} \cdot \mathbf{\Omega}(\mathbf{r}) &= \frac{1}{n(\mathbf{r})}\left[\frac{1}{\Omega_1}\frac{\partial n(\mathbf{r})}{\partial x_1} + \frac{1}{\Omega_2}\frac{\partial n(\mathbf{r})}{\partial x_2} + \frac{1}{\Omega_3}\frac{\partial n(\mathbf{r})}{\partial x_3} - 3\nabla_{\mathbf{r}} n(\mathbf{r}) \cdot \mathbf{\Omega}(\mathbf{r})\right] \\ &= \frac{1}{\Omega_1}\frac{\partial \ln n(\mathbf{r})}{\partial x_1} + \frac{1}{\Omega_2}\frac{\partial \ln n(\mathbf{r})}{\partial x_3} + \frac{1}{\Omega_3}\frac{\partial \ln n(\mathbf{r})}{\partial x_3} - 3\nabla_{\mathbf{r}} \ln n(\mathbf{r}) \cdot \mathbf{\Omega}(\mathbf{r}) \\ &= \nabla_{\mathbf{r}} \ln n(\mathbf{r}) \cdot \mathbf{\Omega}_{\mathrm{inv}}(\mathbf{r}) - 3\nabla_{\mathbf{r}} \ln n(\mathbf{r}) \cdot \mathbf{\Omega}(\mathbf{r}),\end{aligned} \tag{19}$$

where $\mathbf{\Omega}_{\mathrm{inv}}(\mathbf{r}) = \Omega_1^{-1}\hat{\mathbf{x}}_1 + \Omega_2^{-1}\hat{\mathbf{x}}_2 + \Omega_3^{-1}\hat{\mathbf{x}}_3$.

Formula (19) was employed to obtain the Ferwerda final expression for the RTEvri [8], from which a DEvri was derived later by Khan and Jiang [9]. Note that formula (19) only takes into account the effect of the spatial variation of refractive index on the ray divergence and gives a zero ray divergence if the refractive index is constant. Therefore, it ignores that the divergence of rays emerging from a source is different from zero even in a medium of constant refractive index. For example, for an isotropic point source located at the origin of a Cartesian coordinate system in a medium of constant refractive index, the eikonal $\Lambda(\mathbf{r})$, the vector field $\mathbf{\Omega}(\mathbf{r})$ and its divergence $\nabla_{\mathbf{r}} \cdot \mathbf{\Omega}(\mathbf{r})$ are [7]

$$\Lambda(\mathbf{r}) = nr \Rightarrow \mathbf{\Omega}(\mathbf{r}) = \frac{\mathbf{r}}{r} \Rightarrow \nabla_{\mathbf{r}} \cdot \mathbf{\Omega}(\mathbf{r}) = \frac{2}{r} \neq 0, \tag{20}$$

where $r = |\mathbf{r}|$. Therefore, expression (19) fails in this particular case. To avoid this problem we employ a different approach. Using the relation with the eikonal $\Lambda(\mathbf{r})$ (3) we obtain [7]:

$$\nabla_{\mathbf{r}} \cdot \mathbf{\Omega}(\mathbf{r}) = \frac{\nabla_{\mathbf{r}}^2 \Lambda(\mathbf{r})}{n(\mathbf{r})} - \mathbf{\Omega}(\mathbf{r}) \cdot \nabla_{\mathbf{r}} \ln n(\mathbf{r}) = \mu_{\mathrm{d}}(\mathbf{r}) - \nabla_{\mathbf{r}} \ln n(\mathbf{r}) \cdot \mathbf{\Omega}(\mathbf{r}), \tag{21}$$

where $\mu_{\mathrm{d}}(\mathbf{r})$ is the divergence coefficient:

$$\mu_{\mathrm{d}}(\mathbf{r}) = \frac{\nabla_{\mathbf{r}}^2 \Lambda(\mathbf{r})}{n(\mathbf{r})}. \tag{22}$$

From expression (21) it follows that the ray divergence is related to the gradient of refractive index and to the Laplacian of the eikonal, which in turn is related to the wave front shape and, consequently, to the sources of rays. For example, for plane waves propagating in a medium of constant refractive index $\nabla_{\mathbf{r}}{}^2\Lambda(\mathbf{r}) \equiv 0$ and $\nabla_{\mathbf{r}} \ln n(\mathbf{r}) \equiv \mathbf{0}$. It implies $\nabla_{\mathbf{r}} \cdot \mathbf{\Omega}(\mathbf{r}) \equiv 0$, as we could expect. Two things should be highlighted. First, expression (19) cannot be derived from expression (21) and vice versa; it means that these models for the ray divergence are incompatible one with the other. Second, expression (19) presents singularities due to the terms $\Omega_1^{-1}$, $\Omega_2^{-1}$ and $\Omega_3^{-1}$, while expression (21) does not.

Although attractive, the approach based on the expression (21) has some drawbacks. The most important one is that the eikonal is defined for media with no scattering. Consequently, expression (21) ignores the interaction of scattering centers with wave fronts. Another problem is that the eikonal has simple expressions only in a few cases (e.g., for plane wave fronts and spherical wave fronts). New models must be developed to find adequate expressions of the eikonal for more complicated sources and to take into account the effect of scattering centers on wave fronts. In what follows we assume that expression (21) models the ray divergence with enough accuracy and that the coefficient of divergence $\mu_d(\mathbf{r})$ depends only on $\mathbf{r}$.

### 2.3. The term d$\mathbf{\Omega}$/ds

Using expression (5), the property (12) and expression (13) we obtain for the third left-hand term of Eq. (18) [9]:

$$\nabla_{\mathbf{\Omega}} L(\mathbf{r},\mathbf{\Omega},t)\cdot\frac{\mathrm{d}\mathbf{\Omega}}{\mathrm{d}s} = \nabla_{\mathbf{r}} \ln n[\mathbf{R}(s)]\cdot\nabla_{\mathbf{\Omega}} L(\mathbf{R}(s),\mathbf{\Omega},t). \tag{23}$$

### 2.4. The phase function

The phase function describes the fraction of energy transferred from a ray with direction $\mathbf{\Omega}$ to another ray with direction $\mathbf{\Omega}'$ at a point $\mathbf{r}$. The phase function is extremely difficult to assess. Some models as the Henyey–Greenstein function and the Mie kernel for scattering has been used to mathematically represent it [14]. Here we assume that it depends on the scalar product $\Omega\cdot\Omega'$ (scattering independent of the direction of incident photons) and, therefore, can be expanded in a Legendre series of the form [15]:

$$\theta(\mathbf{r},\mathbf{\Omega},\mathbf{\Omega}') = \theta(\mathbf{r},\mathbf{\Omega}\cdot\mathbf{\Omega}') = \frac{1}{4\pi} + \frac{3g(\mathbf{r})}{4\pi}\mathbf{\Omega}\cdot\mathbf{\Omega}' + R_\theta(\mathbf{r},\mathbf{\Omega}\cdot\mathbf{\Omega}'), \tag{24}$$

where $g(\mathbf{r})$ is the asymmetry factor and $R_\theta(\mathbf{r},\mathbf{\Omega}\cdot\mathbf{\Omega}')$ is a remainder that groups orthogonal terms of second order or higher.

Due to the orthogonality of Legendre polynomials the remainder $R_\theta(\mathbf{r},\mathbf{\Omega}\cdot\mathbf{\Omega}')$ has the following properties:

$$\int_{4\pi} R_\theta(\mathbf{r},\mathbf{\Omega}\cdot\mathbf{\Omega}')\,\mathrm{d}\omega = 0, \qquad \int_{4\pi} \mathbf{\Omega} R_\theta(\mathbf{r},\mathbf{\Omega}\cdot\mathbf{\Omega}')\,\mathrm{d}\omega = 0. \tag{25}$$

The assumption of scattering independent of the direction of incident photons seems to fail for structured tissues as muscles [16]. In this paper we limit ourselves to the study of scattering independent of the direction of incident photons.

### 2.5. The Martí–Bouza–Hebden–Arridge–Martínez RTEvri

Substituting the expression (23) in Eq. (18) we obtain the Martí–Bouza–Hebden–Arridge–Martínez RTEvri [7]:

$$\begin{aligned}&\frac{n(\mathbf{r})}{c}\frac{\partial}{\partial t}L(\mathbf{r},\mathbf{\Omega},t) + [\nabla_{\mathbf{r}}\cdot\mathbf{\Omega}(\mathbf{r})]L(\mathbf{r},\mathbf{\Omega},t) + \mathbf{\Omega}(\mathbf{r})\cdot\nabla_{\mathbf{r}}L(\mathbf{r},\mathbf{\Omega},t)\\ &\quad + [\mu_a(\mathbf{r}) + \mu_s(\mathbf{r})]L(\mathbf{r},\mathbf{\Omega},t) + \nabla_{\mathbf{r}}\ln n(\mathbf{r})\cdot\nabla_{\mathbf{\Omega}}L(\mathbf{r},\mathbf{\Omega},t)\\ &\qquad = \mu_s(\mathbf{r})\int_{4\pi}\theta(\mathbf{r},\mathbf{\Omega},\mathbf{\Omega}')L(\mathbf{r},\mathbf{\Omega}',t)\,\mathrm{d}\omega' + \epsilon(\mathbf{r},\mathbf{\Omega},t),\end{aligned} \tag{26}$$

where $\nabla_{\mathbf{r}}\cdot\mathbf{\Omega}(\mathbf{r})$ is given by expression (21). Obviously, for plane waves propagating in a background medium of constant refractive index $\nabla_{\mathbf{r}}\cdot\mathbf{\Omega}(\mathbf{r})\equiv 0$, $\nabla_{\mathbf{r}}\ln n(\mathbf{r})\equiv 0$ and we obtain the time-dependent RTE.

Using the vector identity:

$$[\nabla_{\mathbf{r}}\cdot\mathbf{\Omega}(\mathbf{r})]L(\mathbf{r},\mathbf{\Omega},t) + \mathbf{\Omega}\cdot\nabla_{\mathbf{r}}L\left(\overset{\downarrow}{\mathbf{r}},\mathbf{\Omega},t\right) = \nabla_{\mathbf{r}}\cdot\left[\mathbf{\Omega}(\mathbf{r})L\left(\overset{\downarrow}{\mathbf{r}},\mathbf{\Omega},t\right)\right] \tag{27}$$

and integrating Eq. (26) over a solid angle of 4π sr we obtain the equation [9]:

$$\frac{n(\mathbf{r})}{c}\frac{\partial}{\partial t}I(\mathbf{r},t) + \nabla_{\mathbf{r}}\cdot\mathbf{J}(\mathbf{r},t) + \mu_{\mathrm{a}}(\mathbf{r})I(\mathbf{r},t) + 2\nabla_{\mathrm{r}}\ln n(\mathbf{r})\cdot\mathbf{J}(\mathbf{r},t) = \epsilon_0(\mathbf{r},t), \tag{28}$$

where $I(\mathbf{r}, t)$ is the irradiance and $\mathbf{J}(\mathbf{r}, t)$ is the radiant current density vector, given by the expressions:

$$I(\mathbf{r},t) = \int_{4\pi} L(\mathbf{r},\mathbf{\Omega},t)\,\mathrm{d}\omega, \tag{29}$$

$$\mathbf{J}(\mathbf{r},t) = \int_{4\pi} \mathbf{\Omega}L(\mathbf{r},\mathbf{\Omega},t)\,\mathrm{d}\omega, \tag{30}$$

and $\epsilon_0(\mathbf{r}, t)$ is the power density emitted by the sources:

$$\epsilon_0(\mathbf{r},t) = \int_{4\pi} \epsilon(\mathbf{r},\mathbf{\Omega},t)\,\mathrm{d}\omega. \tag{31}$$

If we integrate Eq. (28) on a convex region $V$ of the medium with its surface $S$ oriented outwards we obtain:

$$\frac{\mathrm{d}}{\mathrm{d}t}W(t) = \int_V \epsilon_0(\mathbf{r},t)\,\mathrm{d}V - \oint_S \mathbf{J}(\mathbf{r},t)\,\mathrm{d}\mathbf{S} - \int_V \mu_{\mathrm{a}}(\mathbf{r})I(\mathbf{r},t)\,\mathrm{d}V - 2\int_V \nabla_{\mathbf{r}}\ln n(\mathbf{r})\cdot\mathbf{J}(\mathbf{r},t)\,\mathrm{d}V, \tag{32}$$

where $W(t)$ is the radiant energy inside $V$

$$W(t) = \int_V \frac{n(\mathbf{r})}{c}I(\mathbf{r},t)\,\mathrm{d}V, \tag{33}$$

$\mathrm{d}V$ is the differential of volume and $\mathrm{d}\mathbf{S}$ is the differential of surface. In the expression (32) we applied the Gauss theorem.

Eqs. (26), (28) and (32) are different expressions of the principle of conservation of energy in the framework of the radiative transfer theory. For example, Eq. (32) links the rate of change of radiant energy inside the volume $V$ with the power emitted by the sources (represented by its first right-hand term), the power that escapes from the volume $V$ (represented by its second right-hand term), the power dissipated inside it (represented by its third right-hand term) and the power spent to change the direction of the rays (represented by its fourth right-hand term). Note also that expressions (28) and (32) are exact.

### *2.6. The time-dependent DEvri*

To derive the DEvri we have to derive the $P_1$ approximation first. We assume that the radiance $L(\mathbf{r},\mathbf{\Omega},t)$ and the source distribution $\epsilon(\mathbf{r},\mathbf{\Omega},t)$ can be expanded in spherical harmonic series of the form:

$$L(\mathbf{r},\mathbf{\Omega},t) = \frac{1}{4\pi}I(\mathbf{r},t) + \frac{3}{4\pi}\mathbf{\Omega}\cdot\mathbf{J}(\mathbf{r},t) + R_L(\mathbf{r},\mathbf{\Omega},t), \tag{34}$$

$$\epsilon(\mathbf{r},\mathbf{\Omega},t) = \frac{1}{4\pi}\epsilon_0(\mathbf{r},t) + \frac{3}{4\pi}\mathbf{\Omega}\cdot\epsilon_1(\mathbf{r},t) + R_\epsilon(\mathbf{r},\mathbf{\Omega},t), \tag{35}$$

where $R_L(\mathbf{r},\mathbf{\Omega},t)$ and $R_\epsilon(\mathbf{r},\mathbf{\Omega},t)$ are remainders that group the terms of the spherical harmonic expansions (34) and (35) of second order or greater, respectively, and the constants 1/(4π) and 3/(4π) are chosen for convenience. Therefore, they have the following properties:

$$\int_{4\pi} R_L(\mathbf{r},\mathbf{\Omega},t)\,\mathrm{d}\omega = 0, \tag{36}$$

$$\int_{4\pi} R_{\epsilon}(\mathbf{r},\mathbf{\Omega},t)\mathrm{d}\omega = 0, \tag{37}$$

$$\int_{4\pi} \mathbf{\Omega} R_L(\mathbf{r},\mathbf{\Omega},t)\,\mathrm{d}\omega = \mathbf{0} \tag{38}$$

$$\int_{4\pi} \mathbf{\Omega} R_{\epsilon}(\mathbf{r},\mathbf{\Omega},t)\,\mathrm{d}\omega = \mathbf{0}. \tag{39}$$

At this point we need to remember that when the operator $\nabla_{\mathbf{r}}$ is applied to the radiance $L(\mathbf{r},\mathbf{\Omega},t)$, it does not act on the direction of propagation $\mathbf{\Omega}(\mathbf{r})$. Obviously, the series (34) inherits this property. For example, we have

$$\begin{aligned}\nabla_{\mathbf{r}} L(\mathbf{r},\mathbf{\Omega}(\mathbf{r}),t) &= \frac{1}{4\pi}\nabla_{\mathbf{r}} I(\overset{\downarrow}{\mathbf{r}},t) + \frac{3}{4\pi}\nabla_{\mathbf{r}}\left[\mathbf{\Omega}(\mathbf{r})\cdot\mathbf{J}(\overset{\downarrow}{\mathbf{r}},t)\right] + \nabla_{\mathbf{r}} R_L(\overset{\downarrow}{\mathbf{r}},\mathbf{\Omega}(\mathbf{r}),t)\\ &= \frac{1}{4\pi}\nabla_{\mathbf{r}} I(\mathbf{r},t) + \frac{3}{4\pi}\left[\Omega_1(\mathbf{r})\nabla_{\mathbf{r}} J_x(\mathbf{r},t) + \Omega_2(\mathbf{r})\nabla_{\mathbf{r}} J_y(\mathbf{r},t) + \Omega_3(\mathbf{r})\nabla_{\mathbf{r}} J_z(\mathbf{r},t)\right] + \nabla_{\mathbf{r}} R_L(\overset{\downarrow}{\mathbf{r}},\mathbf{\Omega},t).\end{aligned} \tag{40}$$

Substituting expansions (34) and (35) in the Eq. (26) we obtain

$$\begin{aligned}&\frac{n(\mathbf{r})}{c}\frac{\partial}{\partial t}\left[\frac{1}{4\pi}I(\mathbf{r},t)+\frac{3}{4\pi}\mathbf{\Omega}\cdot\mathbf{J}(\mathbf{r},t)\right]+[\nabla_{\mathbf{r}}\cdot\mathbf{\Omega}(\mathbf{r})]\left[\frac{1}{4\pi}I(\mathbf{r},t)+\frac{3}{4\pi}\mathbf{\Omega}\cdot\mathbf{J}(\mathbf{r},t)\right]+\frac{1}{4\pi}\mathbf{\Omega}\cdot\nabla_{\mathbf{r}} I(\mathbf{r},t)+\frac{3}{4\pi}\mathbf{\Omega}\cdot\nabla_{\mathbf{r}}\left[\mathbf{\Omega}\cdot\mathbf{J}(\overset{\downarrow}{\mathbf{r}},t)\right]\\ &\quad+[\mu_{\mathrm{a}}(\mathbf{r})+\mu_{\mathrm{s}}(\mathbf{r})]\left[\frac{1}{4\pi}I(\mathbf{r},t)+\frac{3}{4\pi}\mathbf{\Omega}\cdot\mathbf{J}(\mathbf{r},t)\right]+\frac{3}{4\pi}\nabla_{\mathbf{r}}\ln n(\mathbf{r})\cdot\nabla_{\mathbf{\Omega}}[\mathbf{\Omega}\cdot\mathbf{J}(\mathbf{r},t)]+\frac{n(\mathbf{r})}{c}\frac{\partial}{\partial t}R_L(\mathbf{r},\mathbf{\Omega},t)\\ &\quad+[\nabla_{\mathbf{r}}\cdot\mathbf{\Omega}(\mathbf{r})]R_L(\mathbf{r},\mathbf{\Omega},t)+\mathbf{\Omega}\cdot\nabla_{\mathbf{r}} R_L(\overset{\downarrow}{\mathbf{r}},\mathbf{\Omega},t)+[\mu_{\mathrm{a}}(\mathbf{r})+\mu_{\mathrm{s}}(\mathbf{r})]R_L(\mathbf{r},\mathbf{\Omega},t)+\nabla_{\mathbf{r}}\ln n(\mathbf{r})\cdot\nabla_{\mathbf{\Omega}} R_L(\mathbf{r},\mathbf{\Omega},t)\\ &\qquad=\frac{\mu_{\mathrm{s}}(\mathbf{r})}{4\pi}I(\mathbf{r},t)+\frac{3}{4\pi}\int_{4\pi}\theta(\mathbf{r},\mathbf{\Omega},\mathbf{\Omega}')\mathbf{\Omega}'\cdot\mathbf{J}(\mathbf{r},t)\,\mathrm{d}\omega'+\frac{1}{4\pi}\epsilon_0(\mathbf{r},t)+\frac{3}{4\pi}\mathbf{\Omega}\cdot\epsilon_1(\mathbf{r},t)\\ &\qquad\quad+\mu_{\mathrm{s}}(\mathbf{r})\int\theta(\mathbf{r},\mathbf{\Omega},\mathbf{\Omega}')R_L(\mathbf{r},\mathbf{\Omega}',t)\,\mathrm{d}\omega'+R_{\epsilon}(\mathbf{r},\mathbf{\Omega},t).\end{aligned} \tag{41}$$

Multiplying Eq. (41) by $\Omega$**,** integrating the result over a solid angle of $4\pi$ sr and applying properties (38) we obtain the equation:

$$\begin{aligned}&\frac{n(\mathbf{r})}{c}\frac{\partial}{\partial t}\mathbf{J}(\mathbf{r},t)+\underbrace{\frac{1}{4\pi}\int_{4\pi}[\nabla_{\mathbf{r}}\cdot\boldsymbol{\Omega}(\mathbf{r})]I(\mathbf{r},t)\boldsymbol{\Omega}\,\mathrm{d}\omega}_{\mathbf{Q}_1}+\underbrace{\frac{3}{4\pi}\int_{4\pi}[\nabla_{\mathbf{r}}\cdot\boldsymbol{\Omega}(\mathbf{r})]\boldsymbol{\Omega}\cdot\mathbf{J}(\mathbf{r},t)\boldsymbol{\Omega}\,\mathrm{d}\omega}_{\mathbf{Q}_2}\\ &\quad+\underbrace{\frac{1}{4\pi}\int_{4\pi}\boldsymbol{\Omega}\cdot\nabla_{\mathbf{r}} I(\mathbf{r},t)\boldsymbol{\Omega}\,\mathrm{d}\omega}_{\mathbf{Q}_3}+\underbrace{\frac{3}{4\pi}\int_{4\pi}\boldsymbol{\Omega}\cdot\nabla_{\mathbf{r}}\left[\Omega\cdot\mathbf{J}(\overset{\downarrow}{\mathbf{r}},t)\right]\boldsymbol{\Omega}\,\mathrm{d}\omega}_{\mathbf{Q}_4}+[\mu_{\mathrm{a}}(\mathbf{r})+\mu_{\mathrm{s}}(\mathbf{r})]\mathbf{J}(\mathbf{r},t)\\ &\quad+\underbrace{\frac{3}{4\pi}\int_{4\pi}\nabla_{\mathbf{r}}\ln n(\mathbf{r})\cdot\nabla_{\mathbf{\Omega}}[\boldsymbol{\Omega}\cdot\mathbf{J}(\mathbf{r},t)]\boldsymbol{\Omega}\,\mathrm{d}\omega}_{\mathbf{Q}_5}+\underbrace{\int_{4\pi}[\nabla_{\mathbf{r}}\cdot\boldsymbol{\Omega}(\mathbf{r})]R_L(\mathbf{r},\boldsymbol{\Omega},t)\boldsymbol{\Omega}\,\mathrm{d}\omega}_{\mathbf{Q}_6}\\ &\quad+\underbrace{\int_{4\pi}\boldsymbol{\Omega}\cdot\nabla_{\mathbf{r}} R_L(\overset{\downarrow}{\mathbf{r}},\Omega,t)\boldsymbol{\Omega}\,\mathrm{d}\omega}_{\mathbf{Q}_7}+\underbrace{\int_{4\pi}\nabla_{\mathbf{r}}\ln n(\mathbf{r})\nabla_{\mathbf{\Omega}} R_L(\mathbf{r},\boldsymbol{\Omega},t)\boldsymbol{\Omega}\,\mathrm{d}\omega}_{\mathbf{Q}_8}\\ &\qquad=\boldsymbol{\epsilon}_1(\mathbf{r},t)+\underbrace{\frac{3}{4\pi}\int_{4\pi}\boldsymbol{\Omega}\int_{4\pi}\theta(\mathbf{r},\boldsymbol{\Omega},\boldsymbol{\Omega}')\boldsymbol{\Omega}'\cdot\mathbf{J}(\mathbf{r},t)\,\mathrm{d}\omega'\,\mathrm{d}\omega}_{\mathbf{Q}_9}+\underbrace{\mu_{\mathrm{s}}(\mathbf{r})\int_{4\pi}\boldsymbol{\Omega}\int_{4\pi}\theta(\mathbf{r},\boldsymbol{\Omega},\boldsymbol{\Omega}')R_L(\mathbf{r},\boldsymbol{\Omega}',t)\,\mathrm{d}\omega'\,\mathrm{d}\omega}_{\mathbf{Q}_{10}},\end{aligned} \tag{42}$$

where $\mathbf{Q}_1$–$\mathbf{Q}_{10}$ denote terms of interest of Eq. (42).

The terms $\mathbf{Q}_1$–$\mathbf{Q}_5$, $\mathbf{Q}_9$ and $\mathbf{Q}_{10}$ can be calculated. See Appendix A. Further we assume that the terms $\mathbf{Q}_6$, $\mathbf{Q}_7$ and $\mathbf{Q}_8$ meet the following conditions:

$$\mathbf{Q}_6 = \int_{4\pi} [\nabla_{\mathbf{r}} \cdot \mathbf{\Omega}(\mathbf{r})] R_L(\mathbf{r}, \mathbf{\Omega}, t)\mathbf{\Omega}\, \mathrm{d}\omega = -\int_{4\pi} \mathbf{\Omega} \cdot \nabla_{\mathbf{r}} \ln n(\mathbf{r}) R_L(\mathbf{r}, \mathbf{\Omega}, t)\mathbf{\Omega}\, \mathrm{d}\omega \approx \mathbf{0}, \tag{43}$$

$$\mathbf{Q}_7 = \int_{4\pi} \mathbf{\Omega} \cdot \nabla_{\mathbf{r}} R_L(\overset{\downarrow}{\mathbf{r}}, \mathbf{\Omega}, t)\mathbf{\Omega}\, \mathrm{d}\omega \approx \mathbf{0}, \tag{44}$$

$$\mathbf{Q}_8 = \int_{4\pi} \nabla_{\mathbf{r}} \ln n(\mathbf{r}) \cdot \nabla_{\mathbf{\Omega}} R_L(\mathbf{r}, \mathbf{\Omega}, t)\mathbf{\Omega}\, \mathrm{d}\omega \approx \mathbf{0}. \tag{45}$$

Applying conditions (43)–(45) and substituting results (A1)–(A7) into Eq. (42) we obtain:

$$\frac{n(\mathbf{r})}{c}\frac{\partial}{\partial t}\mathbf{J}(\mathbf{r}, t) - \frac{1}{3}[\nabla_{\mathbf{r}} \ln n(\mathbf{r})] I(\mathbf{r}, t) + \frac{1}{3}\nabla_{\mathbf{r}} I(\mathbf{r}, t) + \left[\mu_{\mathrm{a}}(\mathbf{r}) + \mu_{\mathrm{s}}'(\mathbf{r}) + \mu_{\mathrm{d}}(\mathbf{r})\right]\mathbf{J}(\mathbf{r}, t) = \boldsymbol{\epsilon}_1(\mathbf{r}, t), \tag{46}$$

where

$$\mu_{\mathrm{s}}'(\mathbf{r}) = \mu_{\mathrm{s}}(\mathbf{r})[1 - g(\mathbf{r})] \tag{47}$$

is the reduced scattering coefficient.

Eqs. (28) and (46) are the $P_1$ approximation of the Martí–Bouza–Hebden–Arridge–Martínez RTEvri. Eq. (46) differs from the corresponding equation of the $P_1$ approximation obtained by Khan and Jiang [9]. This is a consequence of using expression (21) instead of expression (19) for the divergence term.

To obtain the new time-dependent DEvri we assume that [14]:

$$\boldsymbol{\epsilon}_1(\mathbf{r}, t) \approx \mathbf{0}, \tag{48}$$

$$\frac{\partial}{\partial t}\mathbf{J}(\mathbf{r}, t) \approx \mathbf{0}. \tag{49}$$

Expression (48) means that the source is isotropic and the expression (49) that the variation of the radiant current density vector in time is smooth. Substituting these approximations into Eq. (46) and defining the diffusion coefficient $D(\mathbf{r})$ as:

$$D(\mathbf{r}) = \frac{1}{3\left[\mu_{\mathrm{a}}(\mathbf{r}) + \mu_{\mathrm{s}}'(\mathbf{r}) + \mu_{\mathrm{d}}(\mathbf{r})\right]}, \tag{50}$$

we rewrite Eq. (46) in the form

$$\mathbf{J}(\mathbf{r}, t) = -D(\mathbf{r})\nabla_{\mathbf{r}} I(\mathbf{r}, t) + D(\mathbf{r})[\nabla_{\mathbf{r}} \ln n(\mathbf{r})] I(\mathbf{r}, t). \tag{51}$$

Substituting the latter expression into Eq. (28) we obtain:

$$\frac{n(\mathbf{r})}{c}\frac{\partial}{\partial t} I(\mathbf{r}, t) - \nabla_{\mathbf{r}} \cdot [D(\mathbf{r})\nabla_{\mathbf{r}} I(\mathbf{r}, t)] + \nabla_{\mathbf{r}} \cdot [D(\mathbf{r})\nabla_{\mathbf{r}} \ln n(\mathbf{r}) I(\mathbf{r}, t)] - 2D(\mathbf{r})\nabla_{\mathbf{r}} \ln n(\mathbf{r}) \cdot \nabla_{\mathbf{r}} I(\mathbf{r}, t) + \left[\mu_{\mathrm{a}}(\mathbf{r}) + 2D(\mathbf{r})|\nabla_{\mathbf{r}} \ln n(\mathbf{r})|^2\right] I(\mathbf{r}, t) = \epsilon_0(\mathbf{r}, t). \tag{52}$$

If $\nabla_{\mathbf{r}}^2 \Lambda(\mathbf{r}) \equiv 0$ and $n \equiv$ constant we obtain from equation (52) the standard time dependent DE with the standard diffusion coefficient $D_{\mathrm{std}}(\mathbf{r})$:

$$D(\mathbf{r})|_{\mu_{\mathrm{d}}(\mathbf{r})=0} = D_{\mathrm{std}}(\mathbf{r}) = \frac{1}{3\left[\mu_{\mathrm{a}}(\mathbf{r}) + \mu_{\mathrm{s}}'(\mathbf{r})\right]}. \tag{53}$$

### 2.7. The RTErad and the DErad

If we consider rays of arbitrary divergence, propagating in a medium of constant refractive index ($\mu_d(\mathbf{r}) \not\equiv 0$, $\nabla_\mathbf{r} \ln n(\mathbf{r}) \equiv 0$) we get a particular case of the Martí–Bouza–Hebden–Arridge–Martínez RTEvri (26), the RTE for rays of arbitrary divergence (RTErad). It has the form:

$$\frac{n}{c}\frac{\partial}{\partial t}L(\mathbf{r},\mathbf{\Omega},t) + [\nabla_\mathbf{r}\cdot\mathbf{\Omega}(\mathbf{r})]L(\mathbf{r},\mathbf{\Omega},t) + \mathbf{\Omega}(\mathbf{r})\cdot\nabla_\mathbf{r}L\left(\overset{\downarrow}{\mathbf{r}},\mathbf{\Omega},t\right) + [\mu_a(\mathbf{r}) + \mu_s(\mathbf{r})]L(\mathbf{r},\mathbf{\Omega},t) = \mu_s(\mathbf{r})\int_{4\pi}\theta(\Omega,\Omega')L(\mathbf{r},\mathbf{\Omega}',t)\,\mathrm{d}\omega' + \epsilon(\mathbf{r},\mathbf{\Omega},t). \quad (54)$$

Note that in this case $\mathbf{Q}_6 = \mathbf{Q}_8 = \mathbf{0}$. From Eqs. (28) and (46) we obtain the $P_1$ approximation of the RTErad:

$$\frac{n}{c}\frac{\partial}{\partial t}I(\mathbf{r},t) + \nabla_\mathbf{r}\cdot\mathbf{J}(\mathbf{r},t) + \mu_a(\mathbf{r})I(\mathbf{r},t) = \epsilon_0(\mathbf{r},t), \quad (55)$$

$$\frac{n}{c}\frac{\partial}{\partial t}\mathbf{J}(\mathbf{r},t) + \frac{1}{3}\nabla_\mathbf{r}I(\mathbf{r},t) + \left[\mu_a(\mathbf{r}) + \mu_s'(\mathbf{r}) + \mu_d(\mathbf{r})\right]\mathbf{J}(\mathbf{r},t) = \boldsymbol{\epsilon}_1(\mathbf{r},t). \quad (56)$$

If conditions (48) and (49) hold also, we obtain the DE for rays of arbitrary divergence (DErad):

$$\frac{n}{c}\frac{\partial}{\partial t}I(\mathbf{r},t) - \nabla_\mathbf{r}\cdot[D(\mathbf{r})I(\mathbf{r},t)] + \mu_a(\mathbf{r})I(\mathbf{r},t) = \epsilon_0(\mathbf{r},t). \quad (57)$$

This equation resembles the well-known DE as derived from the standard RTE [14]. The difference is in the diffusion coefficient $D(\mathbf{r})$ (50), which in the DErad contains the divergence coefficient $\mu_d(\mathbf{r})$.

## 3. Isotropic point source in uniform infinite medium

### 3.1. Treatment based on the Martí–Bouza–Hebden–Arridge–Martínez RTEvri

We consider a time-independent isotropic point source located at the coordinate origin. Accordingly the power distribution is described by the expressions:

$$\epsilon_0(\mathbf{r}) = P_0\delta(\mathbf{r}), \quad (58)$$

$$\boldsymbol{\epsilon}_1(\mathbf{r},t) \equiv \mathbf{0}, \quad (59)$$

$$R_\epsilon(\mathbf{r},\mathbf{\Omega},t) \equiv 0. \quad (60)$$

Now we assume that the refractive index, the absorption coefficient and the reduced scattering coefficient are known and constant, and we wish to obtain the irradiance. Consequently, we are dealing with a forward problem. Note also that a constant refractive index implies $\mathbf{Q}_6 = \mathbf{Q}_8 = \mathbf{0}$.

From Eqs. (28) and (46) it follows that:

$$\nabla_\mathbf{r}\cdot\mathbf{J}(\mathbf{r}) + \mu_a I(\mathbf{r}) = P_0\delta(\mathbf{r}), \quad (61)$$

$$\frac{1}{3}\nabla_\mathbf{r}I(\mathbf{r}) + \left[\mu_a + \mu_s' + \frac{2}{r}\right]\mathbf{J}(\mathbf{r}) = \mathbf{0}, \quad (62)$$

where we applied the expression $\mu_d(\mathbf{r}) = 2/r$ (20).

Equivalently, we can transform the time-independent DErad (57) to obtain:

$$-\nabla_{\mathbf{r}} \cdot [D(\mathbf{r})\nabla_{\mathbf{r}} I(\mathbf{r})] + \mu_a I(\mathbf{r}) = P_0 \delta(\mathbf{r}), \tag{63}$$

where $D(\mathbf{r}) = (\mu_a + \mu_s' + 2/r)^{-1}/3$.

### 3.2. Treatment based on the RTE, the Ferwerda–Khan–Jiang RTEvri and the Tualle–Tinet RTEvri

It is easy to show that in a medium with constant refractive index the Ferwerda–Khan–Jiang RTEvri and the Tualle–Tinet RTEvri reduce to the standard RTE. In turn the $P_1$ approximation of the standard RTE and the derived DE are given by Eqs. (61)–(63) with $\mu_d(\mathbf{r}) = 0$ and $D(\mathbf{r}) = D_{std}(\mathbf{r})$. Therefore, we need to solve Eqs. (61) and (62) or, equivalently, Eq. (63), and to take in those solutions $\mu_d(\mathbf{r}) = 0$ and $D(\mathbf{r}) = D_{std}(\mathbf{r})$ to find the solutions to the RTE, the Ferwerda–Khan–Jiang RTEvri and the Tualle–Tinet RTEvri for the specific case of an isotropic point source in an uniform infinite medium.

### 3.3. Symmetry

Firstly, we analyze symmetric properties for vector $\mathbf{r}$. When we move the observation point on a spherical surface centered at the coordinate origin the landscape does not change. Therefore this problem presents radial symmetry and its solution depends on $r = |\mathbf{r}|$. See Fig. 2. Now we analyze the symmetric properties for vector $\mathbf{\Omega}$. At an observation point $\mathbf{r}_0 \neq \mathbf{0}$ the landscape does not change when we rotate the line of sight in the plane perpendicular to $\mathbf{r}_0$. It means that the solution to this problem does not depend on the component of $\mathbf{\Omega}$ perpendicular to $\mathbf{r}_0$. See Fig. 2. For any point $\mathbf{r}_0 \neq \mathbf{0}$ these properties define an axis

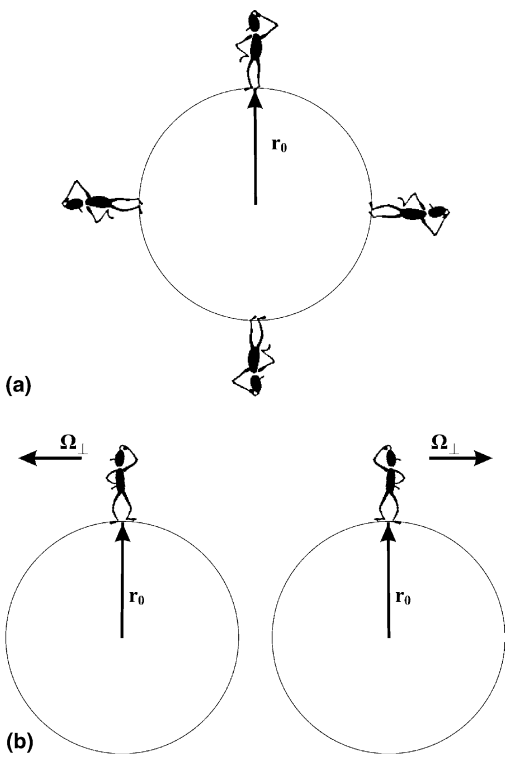


Fig. 2. Symmetric properties.

of symmetry along vector $\mathbf{r}_0$, and a plane of symmetry, which contains point $\mathbf{r}_0$ and is perpendicular to vector $\mathbf{r}_0$ ($\mathbf{\Omega} \cdot \mathbf{r}_0 = 0$). No other axis of symmetry or plane of symmetry can be found for a point $\mathbf{r}_0 \neq \mathbf{0}$. From these symmetric properties it follows that:

$$L(\mathbf{r}, \mathbf{\Omega}) = L(r, \mathbf{\Omega} \cdot \hat{\mathbf{r}}), \tag{64}$$

$$I(\mathbf{r}) = I(r), \tag{65}$$

$$\mathbf{J}(\mathbf{r}) = J(r)\hat{\mathbf{r}}, \tag{66}$$

$$R_L(\mathbf{r}, \mathbf{\Omega}) = R_L(r, \mathbf{\Omega} \cdot \hat{\mathbf{r}}), \tag{67}$$

where $\hat{\mathbf{r}} = \mathbf{r}/r$.

### 3.4. Radiation conditions for a point source at infinity

Since we are dealing with propagation of radiation in an infinite medium it is necessary to impose radiation conditions at infinity. According to the inverse square law of geometrical optics the irradiance from a point source in a non-absorbing non-amplifying no scattering linear medium has the form [13]:

$$I(r) = \frac{\text{constant}}{r^2}. \tag{68}$$

A similar expression for the Poynting vector can be derived from formula (68) using the relation between the irradiance and the Poynting vector in the incoherent case [13]. Therefore, the asymptotic behavior of the irradiance and the radiant current density are of the forms:

$$\lim_{r \to \infty} I(r) \propto \frac{1}{r^2}, \tag{69}$$

$$\lim_{r \to \infty} J(r) \propto \frac{1}{r^2}. \tag{70}$$

A non-zero reduced scattering coefficient should lead to a slower decay of the irradiance because elastic scattering hampers the propagation of light towards infinity, while a non-zero absorption coefficient should cause a faster decay. To illustrate these issues and the expressions (69) and (70) we discuss three trivial cases as follows.

#### 3.4.1. No absorption and no reduced scattering, only divergence effects

Substituting the condition $\mu_a = \mu_s' = 0$ into Eqs. (61) and (62) we obtain the equations:

$$\nabla_{\mathbf{r}} \cdot \mathbf{J}(\mathbf{r}) = P_0 \delta(\mathbf{r}), \tag{71}$$

$$\nabla_{\mathbf{r}} I(\mathbf{r}) = -\frac{6}{r}\mathbf{J}(\mathbf{r}). \tag{72}$$

The solutions to these equations are:

$$I(r) = \frac{3P_0}{4\pi r^2}, \tag{73}$$

$$J(r) = \frac{P_0}{4\pi r^2}. \tag{74}$$

To derive solutions (73) and (74) we applied the Gauss theorem and properties of symmetry. Note that these solutions meet the radiation conditions (69) and (70). It should be noted that in this trivial case the $P_1$ equations of the RTE for an isotropic point source [Eqs. (61) and (62) with $\mu_d = 0$] give the correct expression for the modulus of the radiant current density vector (74), but the wrong irradiance since in Eq. (62) $\mu_d = \mu_a = \mu_s' = 0$ implies $\nabla_{\mathbf{r}} I(r) = 0$ and, consequently, $I(r)$ = constant, a solution that does not meet the radiation condition (69).

*3.4.2. No absorption, non-zero reduced scattering with divergence effect*

Substituting the conditions $\mu_a = 0$ and $\mu_s' =$ constant $\neq 0$ into Eqs. (61) and (62) we obtain the equations:

$$\nabla_{\mathbf{r}} \cdot \mathbf{J}(\mathbf{r}) = P_0 \delta(\mathbf{r}), \tag{75}$$

$$\nabla_{\mathbf{r}} I(\mathbf{r}) = -\left(\mu_s' + \frac{6}{r}\right)\mathbf{J}(\mathbf{r}). \tag{76}$$

The solutions to these equations are:

$$I(r) = \frac{\mu_s' P_0}{4\pi r} + \frac{3P_0}{4\pi r^2}, \tag{77}$$

$$J(r) = \frac{P_0}{4\pi r^2}. \tag{78}$$

From Eq. (77) it follows that the irradiance asymptotic behavior is

$$\lim_{r\to\infty} I(r) \propto \frac{1}{r}. \tag{79}$$

Therefore, its decay is slower than $1/r^2$, as expected. Note that in this case the standard $P_1$ equations of the RTE [Eqs. (61) and (62) with $\mu_d = 0$] for an isotropic point source gives a correct solution for the radiant current density (78) and a solution for the irradiance $I(r) = \mu_s' P_0/(4\pi r)$, which lacks the term $3P_0/(4\pi r^2)$, but has a correct $1/r$ asymptotic behavior. The missing term $3P_0/(4\pi r^2)$ becomes important in the vicinity of the source since it grows faster than $1/r$ as $r \to 0$.

*3.4.3. No scattering, no divergence effect and non-zero absorption*

Substituting condition $\mu_s' = \mu_d = 0$ into equation (63) we obtain the equation:

$$-\frac{1}{3\mu_a}\nabla_{\mathbf{r}}^2 I(\mathbf{r}) + \mu_a I(\mathbf{r}) = P_0 \delta(\mathbf{r}). \tag{80}$$

In spherical coordinates the solution $I(r)$ is:

$$I(r) = \frac{3\mu_a P_0}{4\pi r}\exp\left(-\sqrt{3}\mu_a r\right). \tag{81}$$

Applying Fick's law (62) we obtain the radiant current density:

$$J(r) = -\frac{1}{3\mu_a}\frac{\partial}{\partial r}I(r) = \frac{P_0}{4\pi r^2}\exp\left(-\sqrt{3}\mu_a r\right) + \frac{\sqrt{3}\mu_a P_0}{4\pi r}\exp\left(-\sqrt{3}\mu_a r\right). \tag{82}$$

From expressions (81) and (82) it follows that the asymptotic behaviors are

$$\lim_{r\to\infty} I(r) \to 0, \quad \text{faster than } \frac{1}{r^2}, \tag{83}$$

$$\lim_{r\to\infty} J(r) \to 0, \quad \text{faster than } \frac{1}{r^2}. \tag{84}$$

Therefore, the irradiance decays faster than $1/r^2$, as expected.

### 3.5. Near-field, middle-field and far-field zones

Let us consider three alternative relationships between the coefficients $\mu_a$, $\mu'_s$ and $\mu_d(r)$ as follows:

$$\mu_d(r) \gg \mu_a + \mu'_s, \tag{85}$$

$$\mu_d(r) \sim \mu_a + \mu'_s, \tag{86}$$

$$\mu_d(r) \ll \mu_a + \mu'_s. \tag{87}$$

In the first case (85) we can neglect the coefficients of absorption and reduced scattering in the differential equations (61)–(63); in second case we cannot neglect any of coefficients; and in the third case we can neglect the divergence coefficient.

Now we define a critical radius $R_{crit}$:

$$R_{crit} = \frac{2}{\mu_a + \mu'_s}. \tag{88}$$

We can use this parameter and the expression for the divergence coefficient of a point source (22) in a medium of constant refractive index to identify the relationships (85)–(87) with three zones around the source as follows:

Near field [the inequality (85) is valid]:

$$r \ll R_{crit}. \tag{89}$$

Middle field [neither of inequalities (85) and (87) is valid]:

$$r \sim R_{crit}. \tag{90}$$

Far field [the inequality (87) is valid]:

$$r \gg R_{crit}. \tag{91}$$

The critical radius $R_{crit}$ is a parameter that define the zones where the near-field approximation and the far-field approximation are accurate.

### 3.6. Near-field solution

In near-field $r \ll R_{crit}$ and we can neglect the absorption and reduced scattering coefficients in the expression for the diffusion coefficient $D$ (50). Rewriting the left-hand terms of Eq. (63) in spherical coordinates we obtain:

$$-\frac{r}{6}\frac{d^2 I(r)}{dr^2} - \frac{1}{2}\frac{dI(r)}{dr} + \mu_a I(r) = P_0 \delta(\mathbf{r}). \tag{92}$$

The solution to Eq. (92) is:

$$I(r) = \frac{9P_0\mu_a}{\pi r} K_2\left(2\sqrt{6}\sqrt{\mu_a r}\right), \tag{93}$$

where $K_2(x)$ is a modified Bessel function of second kind.

In the limit $r \to 0$ the function $K_2(2\sqrt{6}\sqrt{\mu_a r})$ can be approximated by the expression $K_2(2\sqrt{6}\sqrt{\mu_a r}) \approx 1/(12\mu_a r)$. Applying this approximation to function (93) we obtain the expression (73). We could expect this result since close enough to a point source the divergence effect predominates over scattering and absorption. We do not need to analyze the behavior of $K_2(2\sqrt{6}\sqrt{\mu_a r})$ as $r \to \infty$ because this solution is not valid for $r > R_{crit}$.

Using Eq. (62) in near-field approximation and applying the properties of symmetry we obtain the radiant current density $J(r)$:

$$J(r) = -\frac{r}{6}\frac{dI(r)}{dr} = P_0\mu_a\frac{\sqrt{6}K_1(2\sqrt{6}\sqrt{\mu_a r}) + 6K_0(2\sqrt{6}\sqrt{\mu_a r})\sqrt{\mu_a r} + 3\sqrt{6}K_1(2\sqrt{6}\sqrt{\mu_a r})\mu_a r}{2\pi r\sqrt{\mu_a r}}, \quad (94)$$

where $K_0(x)$ and $K_1(x)$ are modified Bessel functions of second kind. It is easy to show that in the limit as $r \to 0$ expression (94) yields expression (74).

### 3.7. Far-field solution

In far-field $r \gg R_{crit}$ and we can neglect the divergence coefficient. As a consequence, $D(r) = D_{std}$ and Eq. (63) transforms into the standard DE for an isotropic point source in a uniform infinite medium. Its solution is [4,6]:

$$I(r) = \frac{P_0}{4\pi D_{std} r}\exp\left(-\sqrt{\frac{\mu_a}{D_{std}}}r\right). \quad (95)$$

The radiant current density $J(r)$ is [4,6]:

$$J(r) = -D_{std}\frac{dI(r)}{dr} = \frac{P_0}{4\pi D_{std} r^2}\exp\left(-\sqrt{\frac{\mu_a}{D_{std}}}r\right) + \frac{P_0\sqrt{\mu_a}}{4\pi D_{std}^{3/2} r}\exp\left(-\sqrt{\frac{\mu_a}{D_{std}}}r\right). \quad (96)$$

### 3.8. Comparison with Monte Carlo simulations

The irradiance produced by a time-independent isotropic point source in an uniform infinite medium was simulated by a Monte Carlo code. The code is based on reported descriptions of Monte Carlo codes [4,11,12]. We use a Henyey–Greenstein phase function with $g = 0.8$. The normalized irradiance was calculated at radii up $15R_{crit}$. In Figs. 4–6 the solutions (93), (95) and Monte Carlo simulation results are plotted for following values of parameters: $n = 1$, $\mu_a = 0.01$ mm$^{-1}$, $\mu_s' = 1$ mm$^{-1}$, $R_{crit} = 1.98$ mm; $n = 1$, $\mu_a = 1$ mm$^{-1}$, $\mu_s' = 0.01$ mm$^{-1}$, $R_{crit} = 1.98$ mm; $n = 1$, $\mu_a = 1$ mm$^{-1}$, $\mu_s' = 1$ mm$^{-1}$, $R_{crit} = 1$ mm and $n = 1$, $\mu_a = 0.1$ mm$^{-1}$, $\mu_s' = 0.1$ mm$^{-1}$, $R_{crit} = 10$ mm.

From Figs. 3, 5, 6 it follows that in the region $r < R_{crit}$ the diffusion solution (95) gives highly inaccurate results. This is expected since that solution was obtained for far-field conditions and is not valid in near field. On the other hand, in that region the near-field solution (35) is in good agreement with the results of the Monte Carlo simulation. In the region $r \sim R_{crit}$ (approximately) both solutions yield inaccurate results. This is expected since neither solution is valid within the middle field. Nevertheless, the behavior of the diffusion solutions of the form (95) is better. In the region $r > R_{crit}$ (approximately) the near-field solutions of the form (35) give inaccurate results. Once again this is expected because these solutions are not valid within the far field. The diffusion solutions of the form (95) are in good agreement with the Monte Carlo results.

### 3.9. Inaccuracy of the DE in the vicinity of a point source

Rinzema et al. [3] compared experimentally obtained values of irradiance with the results from the DE and from a rigorous solution of the RTE. From their experimental results a parameter $R_{inacc}$ given by the expression

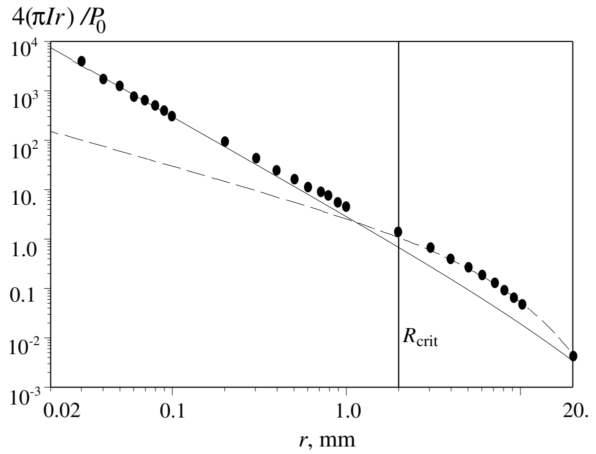


Fig. 3. Plots of normalized near-field (93) and far-field (95) solutions and Monte Carlo results for $n = 1$, $\mu_a = 0.01\text{mm}^{-1}$, $\mu_s' = 1\ \text{mm}^{-1}$ and $R_{crit} = 1.98$ mm. Near field solution $4\pi I(r)/P_0 = 36\mu_a K_2(2\sqrt{6}\sqrt{\mu_a r})/r$ (dash line), far field solution $4\pi I(r)/P_0 = \exp(-\sqrt{\mu_a/D_{std}}r)/(D_{std}r)$ (solid line). Monte Carlo results represented by boxes.

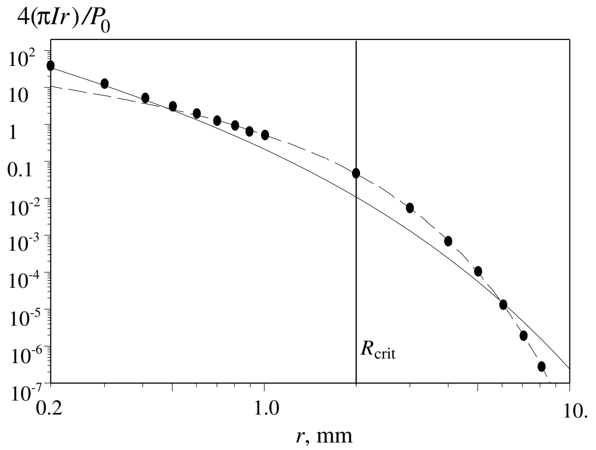


Fig. 4. Plots of normalized near-field (93) and far-field (95) solutions and Monte Carlo results for $n = 1$, $\mu_a = 1\ \text{mm}^{-1}$, $\mu_s' = 0.1\ \text{mm}^{-1}$ and $R_{crit} = 1.98$ mm. Near field solution $4\pi I(r)/P_0 = 36\mu_a K_2(2\sqrt{6}\sqrt{\mu_a r})/r$ (dash line), far field solution $4\pi I(r)/P_0 = \exp(-\sqrt{\mu_a/D_{std}}r)/(D_{std}r)$ (solid line). Monte Carlo results represented by boxes.

$$R_{inacc} = \frac{2}{\mu_a + \mu_s'}, \tag{97}$$

can be defined in order to characterize the region of trust

$$r \gg R_{inacc}, \tag{98}$$

where the DE gives accurate results. In a similar manner, Martelli et al. [4] compared experimentally obtained values of irradiance with results from the DE and from Monte Carlo simulations. From their work it follows that the parameter $R_{inacc}$ is given by:

$$R_{inacc} = \frac{2}{\mu_s'}. \tag{99}$$

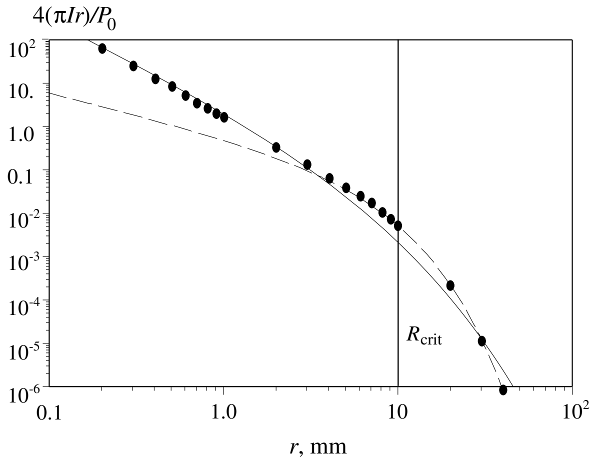


Fig. 5. Plots of normalized near-field (93) and far-field (95) solutions and Monte Carlo results for $n = 1$, $\mu_a = 0.1$ mm $^{-1}$, $\mu_s' = 0.1$ mm$^{-1}$ and $R_{crit} = 10$ mm. Near field solution $4\pi I(r)/P_0 = 36\mu_a K_2(2\sqrt{6}\sqrt{\mu_a r})/r$ (dash line), far field solution $4\pi I(r)/P_0 = \exp(-\sqrt{\mu_a/D_{std}}r)/(D_{std}r)$ (solid line). Monte Carlo results represented by boxes.

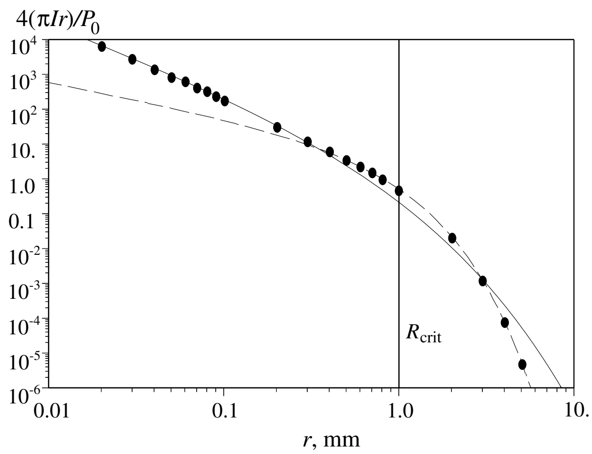


Fig. 6. Plots of normalized near-field (93) and far-field (95) solutions and Monte Carlo results for $n = 1$, $\mu_a = 1$ mm$^{-1}$, $\mu_s' = 0.1$ mm$^{-1}$ and $R_{crit} = 1$ mm. Near field solution $4\pi I(r)/P_0 = 36\mu_a K_2(2\sqrt{6}\sqrt{\mu_a r})/r$ (dash line), far field solution $4\pi I(r)/P_0 = \exp(-\sqrt{\mu_a/D_{std}}r)/(D_{std}r)$ (solid line). Monte Carlo results represented by boxes.

The above expression is a particular case of expression (97) for a weakly absorbing medium. We note that our expression for the critical radius (88) is equal to the above radius of inaccuracy (97):

$$R_{crit} = R_{inacc}. \tag{100}$$

This result suggests that the Rinzema–Murrer–Star condition (98) can be interpreted as a condition for neglecting the divergency of the rays emerging from the point source.

It should be pointed out that our analysis is valid for the use of the DE for forward tasks. For inverse tasks, we need to employ a different approach. Let us suppose that we wish to retrieve the absorption and reduced scattering coefficients $\mu_a \neq 0$ and $\mu_s' \neq 0$ using an algorithm based on the DE. If we impose the Rinzema–Murrer–Star condition (98) (or what is equivalent, $r \gg R_{crit}$) for neglecting the coefficient of divergence $\mu_d$ and ensuring the validity of the DE, then it may occur that:

$$\mu_{\rm a} \lessapprox \mu_{\rm d} \quad \text{or} \quad \mu'_{\rm s} \lessapprox \mu_{\rm d}. \tag{101}$$

Inequalities (101) lead to a paradoxical situation: the neglected parameter $\mu_d$ could be greater than or equal to a parameter to be retrieved ($\mu_a$ or $\mu'_s$) and, consequently, we legitimately can question the accuracy of that retrieved parameter and the validity of the process to retrieve it. We can remove this inconsistency if we require that $\mu_d$ is much less that any of parameters to be retrieved, i.e.

$$\mu_{\rm d} \ll \min[\mu_{\rm a}, \mu'_{\rm s}]. \tag{102}$$

By combining Eq. (20) with the definition of $\mu_d(\mathbf{r})$ (21) and condition (102), we obtain:

$$\frac{2}{r} \ll \min\left[\mu_{\rm a}, \mu'_{\rm s}\right] \Rightarrow r \gg \frac{2}{\min\left[\mu_{\rm a}, \mu'_{\rm s}\right]} = R_{\rm crit}. \tag{103}$$

Note that expression (103) is more 'pessimistic' than expression (97). This is expected because it is derived from a self-consistency criterion for inverse tasks. Note that for most biological tissues in the near infrared region of the light spectrum $\mu_a < \mu'_s$. Therefore, for such media expression (103) adopts the form $R_{crit} = 2/\mu_a$.

## 4. Conclusion

The main results of this work can be summarized as follows.

1. From the Martí–Bouza–Hebden–Arridge–Martínez RTEvri we derived the DEvri (52), the RTErad (54) and the DErad (57).
2. A new diffusion coefficient $D(\mathbf{r})$ (50) was defined. It contains the coefficient of divergence $\mu_d(\mathbf{r})$ and occurs in the DEvri (52) and the DErad (57).
3. For a time-independent isotropic point source in uniform infinite medium we define three different propagation zones, namely, near field ($r \ll R_{crit}$), middle field ($r \sim R_{crit}$), and far-field ($r \gg R_{crit}$). The far-field condition $r \gg R_{crit}$ coincides with the Rinzema–Murrer–Star condition $r \gg R_{inacc}$, defining the zone of accuracy of the DE for this case. This result supports the hypothesis that the inaccuracy of the solutions to the time-independent DE in the vicinity of a point source may be interpreted as due to a missing divergence term in the standard RTE, a problem that the DE inherits. This term occurs in the Martí–Bouza–Hebden–Arridge–Martínez RTEvri and the derived DErad.
4. The far-field solution (for $r \gg R_{crit}$) to the DErad for a time-independent point source in uniform medium (95) is just the solution to the standard time-independent DE equation for the same problem. We could expect this result because in far field the divergence of rays emerging from a point source is negligible.
5. The near-field solution (for $r \ll R_{crit}$) to the DErad was compared with the far-field solutions and with the results of Monte Carlo simulations for three sets parameters of the medium. The good agreement of the near-field solution with the near-field Monte Carlo results strengthens the interpretation of the inaccuracy of the solutions to the DE as due to a missing divergence term.
6. Another estimate for the radius of the region of inaccuracy (103) was derived for inverse problems.

Overall, these results provide strong support for the hypothesis that the failure of the time-independent DE in the vicinity of an isotropic point source can be interpreted as due to an inherent assumption of zero ray divergence in the RTE, a condition that is not met within that region. The Ferwerda–Khan–Jiang RTEvri, the Tualle–Tinet RTEvri and equations derived from them share this drawback because they lack a divergence term or it has an inadequate form. The Martí–Bouza–Hebden–Arridge–Martínez RTEvri and derived equations yield accurate solutions in this case because they contain a term that properly accounts for ray divergence.

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## Appendix A. Calculation of some integrals

$$\mathbf{Q}_1 = \frac{1}{4\pi}\int_{4\pi}[\mu_{\mathrm{d}}(\mathbf{r}) - \mathbf{\Omega}\cdot\nabla_{\mathbf{r}}\ln n(\mathbf{r})]I(\mathbf{r},t)\mathbf{\Omega}\,\mathrm{d}\omega = -\frac{1}{3}\nabla_{\mathbf{r}}\ln n(\mathbf{r})I(\mathbf{r},t), \tag{A1}$$

$$\mathbf{Q}_2 = \frac{3}{4\pi}\int_{4\pi}[\mu_{\mathrm{d}}(\mathbf{r}) - \mathbf{\Omega}\cdot\nabla_{\mathbf{r}}\ln n(\mathbf{r})]\mathbf{\Omega}\cdot\mathbf{J}(\mathbf{r},t)\mathbf{\Omega}\,\mathrm{d}\omega = \mu_{\mathrm{d}}(\mathbf{r})\mathbf{J}(\mathbf{r},t), \tag{A2}$$

$$\mathbf{Q}_3 = \frac{1}{4\pi}\int_{4\pi}\mathbf{\Omega}\cdot\nabla_{\mathbf{r}}I(\mathbf{r},t)\mathbf{\Omega}\,\mathrm{d}\omega = \frac{1}{3}\nabla_{\mathbf{r}}I(\mathbf{r},t), \tag{A3}$$

$$\begin{aligned}\mathbf{Q}_4 &= \frac{3}{4\pi}\int_{4\pi}\mathbf{\Omega}\cdot\nabla_{\mathbf{r}}\left[\mathbf{\Omega}\cdot\mathbf{J}(\overset{\downarrow}{\mathbf{r}},t)\right]\mathbf{\Omega}\,\mathrm{d}\omega = \frac{3}{4\pi}\int_{4\pi}\mathbf{\Omega}\cdot\hat{\mathbf{x}}_1\mathbf{\Omega}\cdot[\nabla_{\mathbf{r}}J_1(\mathbf{r},t)]\mathbf{\Omega}\,\mathrm{d}\omega \\ &\quad + \frac{3}{4\pi}\int_{4\pi}\mathbf{\Omega}\cdot\hat{\mathbf{x}}_2[\mathbf{\Omega}\cdot\nabla_{\mathbf{r}}J_2(\mathbf{r},t)]\mathbf{\Omega}\,\mathrm{d}\omega + \frac{3}{4\pi}\int_{4\pi}\mathbf{\Omega}\cdot\hat{\mathbf{x}}_3[\mathbf{\Omega}\cdot\nabla_{\mathbf{r}}J_3(\mathbf{r},t)]\mathbf{\Omega}\,\mathrm{d}\omega = \mathbf{0},\end{aligned} \tag{A4}$$

where $\mathbf{J}(\mathbf{r},t) = J_1(\mathbf{r},t)\hat{\mathbf{x}}_1 + J_2(\mathbf{r},t)\hat{\mathbf{x}}_2 + J_3(\mathbf{r},t)\hat{\mathbf{x}}_3$.

$$\mathbf{Q}_5 = \frac{3}{4\pi}\int_{4\pi}\{\nabla_{\mathbf{r}}\ln n(\mathbf{r}) - [\nabla_{\mathbf{r}}\ln n(\mathbf{r})\cdot\mathbf{\Omega}]\mathbf{\Omega}\}\cdot\mathbf{J}(\mathbf{r},t)\mathbf{\Omega}\,\mathrm{d}\omega = 0, \tag{A5}$$

$$\begin{aligned}\mathbf{Q}_9 &= \frac{3}{4\pi}\int_{4\pi}\mathbf{\Omega}\int_{4\pi}\theta(\mathbf{\Omega},\mathbf{\Omega}')\mathbf{\Omega}'\cdot\mathbf{J}(\mathbf{r},t)\,\mathrm{d}\omega'\,\mathrm{d}\omega \\ &= \frac{3}{4\pi}\int_{4\pi}\mathbf{\Omega}\int_{4\pi}\left[\frac{1}{4\pi} + \frac{3g(\mathbf{r})}{4\pi}\mathbf{\Omega}\cdot\mathbf{\Omega}' + R_\theta(\mathbf{r},\mathbf{\Omega}\cdot\mathbf{\Omega}')\right]\mathbf{\Omega}'\cdot\mathbf{J}(\mathbf{r},t)\,\mathrm{d}\omega'\,\mathrm{d}\omega \\ &= \frac{3g(\mathbf{r})}{4\pi}\int_{4\pi}\mathbf{\Omega}\mathbf{\Omega}\cdot\mathbf{J}(\mathbf{r},t)\,\mathrm{d}\omega = g(\mathbf{r})\mathbf{J}(\mathbf{r},t),\end{aligned} \tag{A6}$$

$$\begin{aligned}\mathbf{Q}_{10} &= \mu_{\mathrm{s}}(\mathbf{r})\int_{4\pi}\mathbf{\Omega}\int_{4\pi}\theta(\mathbf{\Omega},\mathbf{\Omega}')R_L(\mathbf{r},\mathbf{\Omega}',t)\,\mathrm{d}\omega'\,\mathrm{d}\omega \\ &= \mu_{\mathrm{s}}(\mathbf{r})\int_{4\pi}\mathbf{\Omega}\int_{4\pi}\left[\frac{1}{4\pi} + \frac{3g(\mathbf{r})}{4\pi}\mathbf{\Omega}\cdot\mathbf{\Omega}' + R_\theta(\mathbf{r},\mathbf{\Omega}\cdot\mathbf{\Omega}')\right]R_L(\mathbf{r},\mathbf{\Omega}',t)\,\mathrm{d}\omega'\,\mathrm{d}\omega \\ &= \mu_{\mathrm{s}}(\mathbf{r})g(\mathbf{r})\int_{4\pi}\mathbf{\Omega}\int_{4\pi}\frac{3}{4\pi}\mathbf{\Omega}\cdot\mathbf{\Omega}'R_L(\mathbf{r},\mathbf{\Omega}',t)\,\mathrm{d}\omega'\,\mathrm{d}\omega \\ &\quad + \int_{4\pi}\mathbf{\Omega}\int_{4\pi}R_\theta(\mathbf{r},\mathbf{\Omega}\cdot\mathbf{\Omega}')R_L(\mathbf{r},\mathbf{\Omega}',t)\,\mathrm{d}\omega'\,\mathrm{d}\omega \\ &= \mu_{\mathrm{s}}(\mathbf{r})g(\mathbf{r})\int_{4\pi}\mathbf{\Omega}'R_L(\mathbf{r},\mathbf{\Omega}',t)\,\mathrm{d}\omega' + \int_{4\pi}\left[\int_{4\pi}\mathbf{\Omega}R_\theta(\mathbf{r},\mathbf{\Omega}\cdot\mathbf{\Omega}')\,\mathrm{d}\omega\right]R_L(\mathbf{r},\mathbf{\Omega}',t)\,\mathrm{d}\omega' = \mathbf{0}.\end{aligned} \tag{A7}$$

To calculate above integrals we applied the following identities [17]:

$$\int_{4\pi} \mathbf{\Omega}\,\mathrm{d}\omega = \mathbf{0},$$

$$\int_{4\pi} \mathbf{A}\cdot\mathbf{\Omega}\,\mathrm{d}\omega = 0,$$

$$\int_{4\pi} \mathbf{A}\cdot\mathbf{\Omega}\,\mathbf{\Omega}\,\mathrm{d}\omega = \frac{4\pi}{3}\mathbf{A},$$

$$\int_{4\pi} \mathbf{A}\cdot\mathbf{\Omega}\,\mathbf{B}\cdot\mathbf{\Omega}\,\mathrm{d}\omega = \frac{4\pi}{3}\mathbf{A}\cdot\mathbf{B},$$

$$\int_{4\pi} \mathbf{A}\cdot\mathbf{\Omega}\,\mathbf{B}\cdot\mathbf{\Omega}\,\mathbf{\Omega}\,\mathrm{d}\omega = \mathbf{0}.$$

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