Light propagation at interfaces of biological media: Boundary conditions

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Methods of biomedical optics employed to study and characterize biological media involve measuring light diffusely transmitted though tissue. In this paper we describe boundary conditions for the propagation of light at interfaces of biological media. Boundary conditions are derived for a generalized radiative transfer model that accounts for the propagation of light in biological media with a spatially varying refractive index and includes the effects of ray divergence. This work will improve the accuracy of the measurements in biomedical optics techniques and will enhance our understanding of tissue physiology.

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I. INTRODUCTION

The study and characterization of biological media by optical techniques (like optical imaging and spectroscopy) involve measuring light diffusely transmitted though tissue. Light measurements are usually made at the exterior boundary of the media. Also, the distribution of light in the medium and, therefore, the amount that reaches the exterior boundary are influenced by the interfaces [1]. Thus, the study of the light behavior at the boundaries is mandatory. In this way it is assured that we are really measuring a magnitude corresponding to our model and/or retrieving the correct values of the optical parameters of the media. The propagation of light in biological media is often described within the approach of the radiative transfer theory (RTT), where the standard radiative transfer model is employed [2]. Although the standard radiative transfer model is only valid for media with a uniform refractive index and regions located far from the sources, a generalization of the model has been recently obtained [3]. From now on, we refer to the model that appears in Ref. [3] as the varying refractive index (VRI) model.

The VRI model accounts for the propagation of light in biological media with a spatially varying refractive index and includes the effects of ray divergence. However, no analysis of boundary conditions suitable for the VRI model has yet been reported. In this work, we derive boundary conditions that are appropriate for the VRI model. The boundary conditions are obtained by flux balance equations [4] from which a general formulation can be obtained by expressing the equations as a series of spherical harmonics. This allows approximations to be introduced by selecting a finite set of harmonic terms. Our analysis includes a brief examination of the effect of neglecting higher terms in the spherical harmonic expansion (the "remainder" term). The continuity of the normal component of the radiant current density vector is also demonstrated. Additionally, an expression denoting the so-called "extrapolation distance" is derived. To achieve these results, we take the following steps.

(i) We set the flux balance for a smooth interface by radiance functions.

(ii) We apply the spherical harmonics expansion approximation to the radiance in the flux balance.

(iii) We demonstrate the continuity of the normal component of the radiant current density vector at the boundary for the spherical harmonics expansion approximation.

(iv) We derive a compact boundary condition for the irradiance and the radiant current density where the effect of the remainder is considered.

(v) We obtain a set of diffuse boundary conditions for the VRI model (the condition for the normal component of the radiant current density is included) for a smooth interface.

(vi) We obtain a set of diffuse boundary conditions for the VRI model for a smooth exterior boundary and derive an expression for the extrapolation distance.

II. BOUNDARY CONDITIONS AT A SMOOTH INTERFACE

To derive the diffuse boundary conditions we start from a flux balance at a smooth interface (an analysis of the effect of the roughness of the boundary is beyond the scope of this article) between two biological media [4]. Thus, we consider a smooth boundary δG between two media with spatially varying refractive indices n_1 and n_2 as shown in Fig. 1. The power balance at the interface can be expressed by radiance functions at both sides of the boundary as follows [5,6]:

$$\int_{\mathbf{\Omega}\cdot\mathbf{K}>0} L_1(\mathbf{r},\mathbf{\Omega},t)(\mathbf{K}\cdot\mathbf{\Omega})d\omega = \int_{\mathbf{\Omega}\cdot\mathbf{K}<0} R_{\mathrm{Fresnel}\ 1}L_1(\mathbf{r},\mathbf{\Omega},t)(-\mathbf{K}\cdot\mathbf{\Omega})d\omega + \int_{\mathbf{\Omega}\cdot\mathbf{K}>0}[1-R_{\mathrm{Fresnel}\ 2}]L_2(\mathbf{r},\mathbf{\Omega},t)(\mathbf{K}\cdot\mathbf{\Omega})d\omega, \quad (1)$$

$$\int_{\mathbf{\Omega}\cdot\mathbf{K}<0} L_2(\mathbf{r},\mathbf{\Omega},t)(-\mathbf{K}\cdot\mathbf{\Omega})d\omega = \int_{\mathbf{\Omega}\cdot\mathbf{K}>0} R_{\mathrm{Fresnel}\ 2}L_2(\mathbf{r},\mathbf{\Omega},t)(\mathbf{K}\cdot\mathbf{\Omega})d\omega + \int_{\mathbf{\Omega}\cdot\mathbf{K}<0}[1-R_{\mathrm{Fresnel}\ 1}]L_1(\mathbf{r},\mathbf{\Omega},t)(-\mathbf{K}\cdot\mathbf{\Omega})d\omega, \quad (2)$$

where the vector $\mathbf{K}$ denotes the unit normal to the boundary pointing towards medium 1, the term $L_i(\mathbf{r},\mathbf{\Omega},t)$ denotes the

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radiance at the medium, $i=1,2$, and $R_{\text{Fresnel}i}$ is the angle-dependent Fresnel reflection coefficient for light impinging over the interface from the medium, $i=1,2$ [7].

We then assume that the radiance functions at both sides of the boundary can be expanded in a series of spherical harmonics of the formula

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

where $I(\mathbf{r},t)$ and $\mathbf{J}(\mathbf{r},t)$ are the irradiance and the radiant current density vector, respectively, and the remainder $R_L(\mathbf{r},\mathbf{\Omega},t)$ groups the second- and higher-order terms of the expansion [8]. If only N terms are considered in the expansion (3), we are dealing with a P_N approximation and the effect of the remainder should appear at the boundary conditions.

By substituting Eq. (3) into Eqs. (1) and (2) and combining the results we can derive an expression for the normal component of the radiant current density vector (see Appendix A):

$$J_{1\mathbf{K}}(\mathbf{r},t) = J_{2\mathbf{K}}(\mathbf{r},t), \quad \mathbf{r}\in\delta G, \quad (4)$$

where $J_{i\mathbf{K}}(\mathbf{r},t)=\mathbf{J}_i(\mathbf{r},t)\cdot\mathbf{K}$. Equation (4) expresses the continuous character of the normal component of the radiant current density vector at the boundary of the media. This boundary condition is valid for any order of the series (3) and, consequently, is also valid for the diffusion approximation.

With a similar procedure as described to derive expression (4) (see Appendix A for details about the common procedure) we can also obtain a compact boundary condition for $I(\mathbf{r},t)$ and $\mathbf{J}(\mathbf{r},t)$ at both media as follows:

$$[1-R_{I_1}]\frac{I_1(\mathbf{r},t)}{2} + [R_{J_1}+R_{J_2}]J_{\mathbf{K}}(\mathbf{r},t) - [1-R_{I_2}]\frac{I_2(\mathbf{r},t)}{2}$$
$$= 2\int_{\mathbf{\Omega}\cdot\mathbf{K}<0} R_{\text{Fresnel }1}(-\mathbf{K}\cdot\mathbf{\Omega})R_{L_1}(\mathbf{r},\mathbf{\Omega},t)(\mathbf{K}\cdot\mathbf{\Omega})d\omega$$
$$- 2\int_{\mathbf{\Omega}\cdot\mathbf{K}>0} R_{\text{Fresnel }2}(\mathbf{K}\cdot\mathbf{\Omega})R_{L_2}(\mathbf{r},\mathbf{\Omega},t)(\mathbf{K}\cdot\mathbf{\Omega})d\omega, \quad (5)$$
$$\mathbf{r}\in\delta G,$$

where we used Eq. (4) and where $J_{\mathbf{K}}(\mathbf{r},t)=\mathbf{J}_{\mathbf{K}}(\mathbf{r},t)\cdot\mathbf{K}$ denotes the normal component of the radiant current density vector at the boundary. Expression (5) gives the boundary condition for the discontinuity of the irradiance without excluding the contribution of the higher-order terms of the spherical harmonic expansion. Note that the boundary condition given by Eq. (5) links the remainder with the irradiance and the radiant current density vector. Consequently, neglecting the effect of the remainder affects the values of the irradiance and the radiant current density vector at the boundary condition and, thus, their profile at the media.

In the P_1 approximation, the effect of the remainder in Eq. (3) is neglected and we obtain the following expression for Eq. (5):

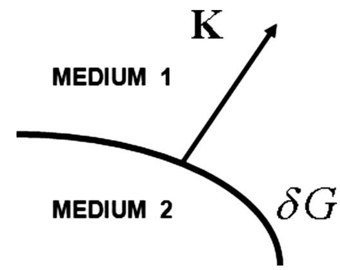

FIG. 1. Scheme of the boundary.

$$I_2(\mathbf{r},t) - \left(\frac{n_2}{n_1}\right)^2 I_1(\mathbf{r},t) = 2\frac{R_{J_1}+R_{J_2}}{1-R_{I_1}}J_{\mathbf{K}}(\mathbf{r},t), \quad \mathbf{r}\in\delta G, \quad (6)$$

where we introduced the relation

$$n_1^2[1-R_{\text{Fresnel }1}] = n_2^2[1-R_{\text{Fresnel }2}], \quad (7)$$

derived from Snell's law [9].

In the diffusion approximation of the VRI model, the radiant current density vector is related to the irradiance according to the expression [3]

$$\mathbf{J}(\mathbf{r},t) = -D(\mathbf{r})\nabla_{\mathbf{r}}I(\mathbf{r},t) + D(\mathbf{r})\nabla_{\mathbf{r}}\ln n(\mathbf{r})I(\mathbf{r},t), \quad (8)$$

where

$$D(\mathbf{r}) = \frac{1}{3[\mu_a(\mathbf{r})+\mu_s'(\mathbf{r})+\mu_d(\mathbf{r})]} \quad (9)$$

is the diffusion coefficient and μ_a, μ_s', and μ_d are the absorption, reduced scattering, and divergence coefficients, respectively. The divergence coefficient μ_d is related to the wavefront shape and, consequently, to the sources of rays [3]. This term plays a crucial role in describing the propagation of light near the sources and does not appear in the diffusion equation derived from the standard radiative transfer model [2].

Furthermore, note that Eq. (8) is not the classical Fick's law due to the linear dependence of the radiant current density vector on the irradiance. If we substitute expression (8) into (4) we will finally obtain

$$-D_1(\mathbf{r})\frac{\partial I_1(\mathbf{r},t)}{\partial K} + D_1(\mathbf{r})\frac{\partial \ln n_1(\mathbf{r})}{\partial K}I_1(\mathbf{r},t)$$
$$= -D_2(\mathbf{r})\frac{\partial I_2(\mathbf{r},t)}{\partial K} + D_2(\mathbf{r})\frac{\partial \ln n_2(\mathbf{r})}{\partial K}I_2(\mathbf{r},t), \quad (10)$$

where the operator $\partial/\partial K=\mathbf{K}\cdot\nabla_{\mathbf{r}}$ represents the directional derivate along $\mathbf{K}$. On finding the irradiance, Eqs. (6) and (10) must be used simultaneously.

III. BOUNDARY CONDITIONS AT AN EXTERIOR BOUNDARY

In case of a biological medium-air interface (exterior boundary), very common in geometries of characterization of biological media and medical treatment and diagnosis, instead of expressions (1) and (2) we have to use

$$\int_{\mathbf{\Omega}\cdot\mathbf{K}<0}(-\mathbf{K}\cdot\mathbf{\Omega})L(\mathbf{r},\mathbf{\Omega},t)d\omega = \int_{\mathbf{K}\cdot\mathbf{\Omega}>0}R_{\text{Fresnel}}(\mathbf{K}\cdot\mathbf{\Omega})L(\mathbf{r},\mathbf{\Omega},t)(\mathbf{K}\cdot\mathbf{\Omega})d\omega, \quad \mathbf{r}\in\delta G. \tag{11}$$

Following the same reasoning that led to former equations we find the following expression:

$$I(\mathbf{r},t)\left\{1-2R_{\text{eff}}D(\mathbf{r})\frac{\partial\ln n(\mathbf{r})}{\partial K}\right\}+2R_{\text{eff}}D(\mathbf{r})\frac{\partial I(\mathbf{r})}{\partial K}=0, \tag{12}$$

$$\mathbf{r}\in\delta G,$$

where expression (4) holds and $R_{eff}=(1+R_{\mathbf{J}})/(1-R_{I})$ is an effective Fresnel coefficient. Details concerning R_{eff} and expression (12) derivation can be found in Appendix B. Expression (11) is a mixed Dirichlet-Neuman boundary condition, and it is similar to the Robin boundary condition [10]. This formula can be used to obtain the extrapolation distance d, which is a magnitude characterizing the diffusion process of light at the biological medium usually known from the Milne problem [1].

In the standard radiative transfer model, $d_{\text{std}}=2R_{\text{eff}}D_{\text{std}}$, where $D_{std}=\{3[\mu_{\text{a}}(\mathbf{r})+\mu_{\text{s}}'(\mathbf{r})]\}^{-1}$ is the standard diffusion coefficient. Thus, according to the definition of the extrapolation distance and expression (11) we obtain a new value for the extrapolation distance d:

$$d=\frac{2R_{\text{eff}}D(\mathbf{r})}{1-2R_{\text{eff}}D(\mathbf{r})[\partial\ln n(\mathbf{r})/\partial K]}, \quad \mathbf{r}\in\delta G. \tag{13}$$

Note that even in the presence of a medium with a constant refractive index and a matched exterior boundary ($R_{\text{eff}}=1$), expression (12) differs from the standard value of the extrapolation distance. This difference becomes important when the source is embedded in the medium and located near the boundary such as, for example, in medical treatment of skin cancer where the absorption beneath the skin by the tumor is considerable. To analyze this situation, the irradiance produced by a time-independent isotropic point source in a uniform infinite medium was simulated by a Monte Carlo code for several sets of optical parameters: $\mu_{\text{a}}=(0.01;0.1;1)\ \text{mm}^{-1}$ and $\mu_{\text{s}}'=(1;0.01;0.1)\ \text{mm}^{-1}$. The code is based on a reported description of the Monte Carlo code [11].

The values of the optical parameters and the source positioning allows us to recreate a situation where the standard diffusion equation fails to describe light propagation [12,13]. In this case the diffusion equation derived from the VRI model has not the usual constraints on the absorption and scattering coefficients and describes the propagation of light up to very near the source with good accuracy [3].

Finally, we corroborated that the theoretical value of the extrapolation distance in the aforementioned situation can be calculated to any desirable accuracy by the expression

$$d\approx d^{(N)}=\frac{1}{3}\sum_{k=0}^{N}(-1)^{k}\left(\frac{\mu_{\text{a}}+\mu_{\text{s}}'}{2}\right)^{k}r_{0}^{k+1}, \tag{14}$$

where r_0 is the minimal distance to the boundary and the degree of the accuracy of the calculation of d can be increased by the order of the series, N.

IV. CONCLUSIONS

In this paper we derived boundary conditions for a generalized radiative transfer model that describe light propagation in media with a spatially varying refractive index and arbitrary ray divergence (the VRI model). The results can be summarized by grouping the expressions of the boundary conditions according to the position of the boundary in the media and the type of the approximation.

For a smooth interface between two diffusive media, expressions (4) and (5) are boundary conditions valid for the spherical harmonics expansion approximation (3). Equation (4) expresses the continuous character of the normal component of the radiant current density vector. Expression (5) allows quantifying the discontinuity of the irradiance without neglecting the effect of the remainder term. In the P_1 approximation expression (5) should be replaced by (6). Furthermore, in the diffusion approximation, the normal component of the radiant current density vector can be related to the irradiance by expression (8). The corrections for the spatial variation of the refractive index and the ray divergence effects appear explicitly in the formulas by the introduction of the gradient of the refractive index function and the diffusion coefficient (9).

For an exterior boundary, the power balance can be expressed by expression (11) instead of expressions (1) and (2). In this case, the boundary condition for the diffusion approximation takes the form of expression (12). The former expression leads to a new value for the extrapolation distance which can be used to obtain information about the optical parameters of a medium—for example, tissues.

Finally, we expect that the use of these boundary conditions increases the accuracy of measurements in biomedical optics techniques, improves spatial resolution in optical imaging and spectroscopy, and enhances our understanding of physiology and biological media in general.

APPENDIX A: BOUNDARY CONDITION AT A SMOOTH INTERFACE AND CONTINUITY OF THE RADIANT CURRENT DENSITY VECTOR

The direct substitution of the series of spherical harmonics (3) into expressions (1) and (2) yields

$$\frac{I_1(\mathbf{r},t)}{4}(1-R_{I_1})+\frac{J_{1\mathbf{K}}(\mathbf{r},t)}{2}(1+R_{\mathbf{J}_1})+\int_{\mathbf{\Omega}\cdot\mathbf{K}>0}R_{L_1}(\mathbf{r},\mathbf{\Omega},t)(\mathbf{K}\cdot\mathbf{\Omega})d\omega$$
$$=\int_{\mathbf{\Omega}\cdot\mathbf{K}<0}R_{L_1}(\mathbf{r},\mathbf{\Omega},t)R_{\text{Fresnel }1}(-\mathbf{K}\cdot\mathbf{\Omega})d\omega+\frac{I_2(\mathbf{r},t)}{4}(1-R_{I_2})+\frac{J_{2\mathbf{K}}(\mathbf{r},t)}{2}(1-R_{\mathbf{J}_2})+\int_{\mathbf{\Omega}\cdot\mathbf{K}>0}R_{L_2}[1-R_{\text{Fresnel }2}(\mathbf{K}\cdot\mathbf{\Omega})]$$
$$\times(\mathbf{K}\cdot\mathbf{\Omega})d\omega, \tag{A1}$$

$$\mathbf{r}\in\delta G,$$

$$\frac{I_2(\mathbf{r},t)}{4}(1-R_{I_2})-\frac{J_{2\mathbf{K}}(\mathbf{r},t)}{2}(1+R_{\mathbf{J}_2})+\int_{\mathbf{\Omega}\cdot\mathbf{K}<0}R_{L_2}(\mathbf{r},\mathbf{\Omega},t)(-\mathbf{K}\cdot\mathbf{\Omega})d\omega$$
$$=\int_{\mathbf{\Omega}\cdot\mathbf{K}>0}R_{L_2}(\mathbf{r},\mathbf{\Omega},t)R_{\text{Fresnel }2}(\mathbf{K}\cdot\mathbf{\Omega})d\omega+[1-R_{I_1}]\frac{I_1(\mathbf{r},t)}{4}-[1-R_{J_1}]\frac{J_{1\mathbf{K}}(\mathbf{r},t)}{2}+\int_{\mathbf{\Omega}\cdot\mathbf{K}<0}R_{L_1}(\mathbf{r},\mathbf{\Omega},t)[1-R_{\text{Fresnel }1}(\mathbf{K}\cdot\mathbf{\Omega})]$$
$$\times(\mathbf{K}\cdot\mathbf{\Omega})d\omega, \tag{A2}$$

$$\mathbf{r}\in\delta G,$$

where $J_{i\mathbf{K}}(\mathbf{r},t)$, $i=1,2$, is the normal component of the radiant current density vector and the coefficients R_{I_i} and $R_{\mathbf{J}_i}$, $i=1,2$, can be calculated for each medium by the following expressions:

$$R_I=2\int_0^1 xR_{Fresnel}(x)dx, \tag{A3}$$

$$R_J=3\int_0^1 x^2R_{Fresnel}(x)dx. \tag{A4}$$

It should be noted that due to the orthogonality of the spherical harmonic terms, the remainders appearing in expressions (A1) and (A2) have the following properties:

$$\int_{4\pi}R_L(\mathbf{r},\mathbf{\Omega},t)d\omega=0, \tag{A5}$$

$$\int_{4\pi}\mathbf{\Omega}R_L(\mathbf{r},\mathbf{\Omega},t)d\omega=0. \tag{A6}$$

If we combine Eqs. (A1) and (A2) and take into account the properties of the remainders expressed in Eqs. (A5) and (A6), after some rearrangement we will obtain

$$J_{1\mathbf{K}}(\mathbf{r},t)=J_{2\mathbf{K}}(\mathbf{r},t),\quad \mathbf{r}\in\delta G. \tag{A7}$$

APPENDIX B: BOUNDARY CONDITION AT AN EXTERIOR BOUNDARY

We need to calculate

$$\int_{\mathbf{\Omega}\cdot\mathbf{K}<0}L(\mathbf{r},\mathbf{\Omega})(\mathbf{\Omega}\cdot-\mathbf{K})d\omega$$
$$=\int_{\mathbf{\Omega}\cdot\mathbf{K}>0}R_{Fresnel}(\mathbf{\Omega}\cdot\mathbf{K})L(\mathbf{r},\mathbf{\Omega})(\mathbf{\Omega}\cdot\mathbf{K})d\omega. \tag{B1}$$

The substitution of the series of spherical harmonics (6) into Eq. (B1) yields

$$\frac{1}{4}I(\mathbf{r},t)(1-R_I)-\frac{1}{2}[\mathbf{J}(\mathbf{r},t)\cdot\mathbf{K}](1+R_J)$$
$$+\int_{\mathbf{\Omega}\cdot\mathbf{K}<0}R_L(\mathbf{r},\mathbf{\Omega},t)(\mathbf{\Omega}\cdot-\mathbf{K})d\omega$$
$$=\int_{\mathbf{\Omega}\cdot\mathbf{K}>0}R_{Fresnel}(\mathbf{\Omega}\cdot\mathbf{K})R_L(\mathbf{r},\mathbf{\Omega},t)(\mathbf{\Omega}\cdot\mathbf{K})d\omega, \tag{B2}$$

where the coefficients R_I and $R_{\mathbf{J}}$ can be calculated for each medium by expressions (A3) and (A4). If we neglect the effect of the remainders (P_1 approximation), we obtain

$$\frac{1}{4}I(\mathbf{r},t)(1-R_I)-\frac{1}{2}[\mathbf{J}(\mathbf{r},t)\cdot\mathbf{K}](1+R_J)=0. \tag{B3}$$

If we define the operator $\partial/\partial K=\mathbf{K}\cdot\mathbf{\nabla_r}$ and the effective Fresnel coefficient R_{eff},

$$R_{eff}=(1+R_{\mathbf{J}})/(1-R_I). \tag{B4}$$

Then, by substitution, we will obtain

$$I(\mathbf{r},t)\left\{1-2R_{\text{eff}}D(\mathbf{r})\frac{\partial\ln n(\mathbf{r})}{\partial K}\right\}+2R_{\text{eff}}D(\mathbf{r})\frac{\partial I(\mathbf{r})}{\partial K}=0,$$
$$\mathbf{r}\in\delta G. \tag{B5}$$

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