Analytic evaluation of diffuse flux at a refractive index discontinuity in forward-biased scattering media

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ABSTRACT

A simple analytic method of estimating the error involved in using an approximate boundary condition for diffuse radiation in two adjoining scattering media with differing refractive index is presented. The method is based on asymptotic planar fluxes and enables the error to be readily evaluated without recourse to Monte Carlo simulation. The analysis is extended to multi-layer media, for which the cumulative error can exceed 100% when an approximate boundary condition is used.

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The boundary condition at an interface between two diffusive scattering media with differing refractive indices n_1, n_2 involves a discontinuity in the scalar flux φ proportional to the magnitude of the vector flux J at the boundary, which is conserved across the interface [1-4]

$$n^2\varphi_1 - \varphi_2 = C(n)J \qquad (1)$$

where $n = n_2/n_1 > 1$ and the proportionality constant $C(n) \propto (n-1)^{3/2}$ for $n-1 \ll 1$ [1]. Hence $n^2\varphi_1 > \varphi_2$ when $J>0$. The error in applying the simpler boundary condition [5]

$$n^2\varphi_1 - \varphi_2 = 0 \qquad (2)$$

has been investigated numerically for biological tissue [3] and analytically for time-dependent diffusion between adjacent half-spaces [6]. Most analyses employ a point source located a finite distance from the surface boundary (Green's function solution), which therefore appears as a parameter in the result, and minimal or zero absorption and isotropic or moderately anisotropic scattering (as required by diffusion theory). Here we present a simpler approach based on the asymptotic diffuse flux to derive a general analytic result determined solely by the boundary conditions at an interface and the inherent optical properties of the scattering media, enabling rapid evaluation of the error.

With the definitions

$$\varphi = ½ \int I(\mu)d\mu \qquad \mu \in |-1, 1| \qquad (3a)$$

$$J = ½ \int I(\mu)\mu d\mu \qquad \mu \in |-1, 1| \qquad (3b)$$

where $I(\mu)$ is the angular intensity distribution and μ the direction cosine, we find the mean cosine of the radiance $<\mu> = \int I(\mu)\mu d\mu / \int I(\mu)d\mu = J/\varphi$. Dividing eqn (1) by φ_1, we find the fractional error in applying the approximate boundary condition eq (2)

$$\Delta\varphi/\varphi_1 = n^2 - \varphi_2/\varphi_1 = C(n)<\mu_1> \qquad (4a)$$

And similarly

$$\Delta\varphi/\varphi_2 = n^2\varphi_1/\varphi_2 - 1 = C(n)<\mu_2> \qquad (4b)$$

Thus the error in applying the approximate boundary condition eqn (2) is directly proportional to the mean cosine $<\mu>$ of the angular intensity distribution at the boundary. The discontinuity in scalar flux φ quantified by eqn (1) also implies a discontinuity in the mean cosine $<\mu>$ of the radiance distribution viz. $<\mu_1> \neq <\mu_2>$. To find the magnitude of the error in a specific case requires numerical evaluation of the boundary fluxes [3]. However, a preliminary estimate can be made in terms of the mean cosine of the asymptotic angular radiance [7]

$$<\mu>_{as} = (1 - \omega_0)/\gamma_0 \qquad (5)$$

for scattering albedo $\omega_0 = \kappa_s/(\kappa_s+\kappa_a) = \kappa_s/\kappa_e$, where κ_s is the scattering coefficient, κ_a the absorption coefficient, $\kappa_e = \kappa_s+\kappa_a$ the extinction coefficient and γ_0 the least eigenvalue of the scattering matrix [8], equivalent to the diffuse attenuation coefficient κ_d. In the P1 approximation, κ_d and $<\mu>_{as}$ are determined solely by κ_s, κ_a and scattering asymmetry g

$$\kappa_d = [3\kappa_a(\kappa_a + \kappa_s')]^{1/2} \approx \sqrt{(3\kappa_a\kappa_s')} \qquad (6a)$$

$$<\mu>_{as} = [\kappa_a/3(\kappa_a + \kappa_s')]^{1/2} \approx \sqrt{(\kappa_a/3\kappa_s')} \quad (6b)$$

when $\kappa_a \ll \kappa_s'$, with $\kappa_s' = \kappa_s(1-g)$ [9]. Thus $\kappa_d \Rightarrow 0$, $<\mu>_{as} \Rightarrow 0$ when $\kappa_a \Rightarrow 0$ (zero absorption). More precise evaluation of the eigenvalue γ_0 (and hence κ_d) required for forward-biased scattering in absorbing media, involves higher moments of the phase function [10, 11].

The dependence of the error $\Delta\varphi/\varphi$ on scattering asymmetry g is shown in Fig 1 for scattering albedoes in the range $\varpi_0 \in |0.2\text{-}0.99|$ (for accurate values of γ_0 [10, 11]). It can be seen that $\Delta\varphi/\varphi$ is only weakly dependent on scattering asymmetry for g<0 (backward-biased scattering), even for strong absorption ($\varpi_0 = 0.2$ i.e. $\kappa_a = 4\kappa_s$), while increasing rapidly for forward-biased scattering (g>0), approaching 10% for g≥0.99 when ϖ_0=0.9. In the δ-P1 approximation, the scattering asymmetry is reduced: $g' \in |0, 0.5|$ for $g \in |0, 1|$, but so is the scattering albedo: $\varpi_0' = \kappa_s'/(\kappa_s'+\kappa_a)$ via the reduced scattering coefficient $\kappa_s' = \kappa_s(1\text{-}g)$. Thus for g = 0.9, rescaling increases the effective absorption *tenfold*, potentially offsetting the reduced error in φ. The error in the diffuse flux increases for interfaces with higher index ratios, $\Delta\varphi/\varphi$ exceeding 20% for g = 0.95 when n = 1.25 (ϖ_0 = 0.99).

To proceed further, we require solutions of the diffusion equation for two adjoining layers satisfying the boundary condition eqn (1). To simplify the analysis, we consider planar asymptotic solutions for φ_1 and φ_2 in the respective scattering media [12]

$$\varphi_1(z) = a_1\exp(\kappa_1 z) + b_1\exp(-\kappa_1 z) \qquad z<0 \qquad (7a)$$

$$\varphi_2(z) = a_2\exp(\kappa_2 z) + b_2\exp(-\kappa_2 z) \qquad z>0 \qquad (7b)$$

with diffuse attenuation coefficients κ_1, κ_2, taking the z-axis perpendicular to the interface at z = 0. Applying the boundary condition eqn (1) and defining $J = -D\nabla\varphi$, where D is the diffusion coefficient, and setting $J_1(0) = J_2(0)$ [1], we find

$$\varphi_1(0) = 2K/1+K \qquad (8a)$$

$$\varphi_2(0) = 2D_1\kappa_1/D_2\kappa_2(1+K) \qquad (8b)$$

where $$K = [D_1\kappa_1/n^2D_2\kappa_2][1+C(n)D_2\kappa_2] \qquad (8c)$$

assuming a semi-infinite medium (half-space) for z>0: $a_2 = 0$ for $\varphi_2(z)\Rightarrow 0$ as $z\Rightarrow\infty$.

Eqns (8a,b,c) enable comparison of the diffuse boundary fluxes $\varphi_1(0)$, $\varphi_2(0)$ with those satisfying the approximate boundary condition eq (2), which follow on setting C(n) = 0. Analytic evaluation of the fractional flux error in terms of the refractive index ratio $n=n_2/n_1$ and the diffusion parameters $D_1\kappa_1$, $D_2\kappa_2$ via the scattering asymmetry g and scattering albedo ω_0 can then be made. Accurate values of $D_1\kappa_1$ and $D_2\kappa_2$ for forward-biased anisotropic scattering in absorbing media (ω_0<1) may be calculated from the phase function $p(\mu)$ and scattering albedo ω_0 [10, 11]. Alternatively, the mean cosine $<\mu>_{as}$ of the asymptotic radiance can be obtained from eq (5) and used in place of $D\kappa$. Only the eigenvalue γ_0 need be calculated in this case, analytically in the P1 or P3 approximations [13, 14], or numerically for higher accuracy.

Fig. 2 shows the dependence of the fractional errors in the diffuse fluxes vs. scattering albedo ϖ_0 for two adjoining media with disparate scattering parameters (g = 0, 0.95), calculated in the P1 and P3 approximations to the diffusion parameters for Henyey-Greenstein scattering [15], with refractive index ratio n = 1.41/1.34 = 1.06 (tissue/aq). Initially, the error increases rapidly with absorption (ϖ_0<1) for g = 0.95, with a broad maximum $\Delta\varphi/\varphi \sim 6\%$ for $\varpi_0 \sim 0.6$; in contrast, the error for isotropic scattering (g = 0) in the adjoining medium increases quasi-linearly to ~ 5% when $\varpi_0 = 0$. The results show that the P1 approximation seriously underestimates the error in diffuse flux (by ~40%), while P3 is ≤10% low compared with the accurate value (P99), and is preferred for analytic evaluation of $\Delta\varphi/\varphi$. Overall the results show that the error increases sharply when there is non-negligible absorption in a scattering medium with strongly forward biased scattering.

More generally, for diffusion of light in multiple layers of finite thickness, the diffuse flux $\varphi_k(z)$ in the kth layer may be expressed as [12]

$$\varphi_k(z) = a_k\exp(\kappa_k z) + b_k\exp(-\kappa_k z) \qquad (9)$$

with a similar expression for $\varphi_{k+1}(z)$ in the (k+1)th layer. The boundary conditions [3, 4]

$$(n_{k+1}/n_k)^2\varphi_k(z_k) - \varphi_{k+1}(z_k) = C(n_{k+1}/n_k)J_k(z_k) \qquad (10a)$$

$$J_k(z_k) = J_{k+1}(z_k) : D_k\nabla\varphi_k(z_k) = D_{k+1}\nabla\varphi_{k+1}(z_k) \qquad (10b)$$

yield the simple recurrence relations (for $n = n_{k+1}/n_k > 1$)

$$a_{k+1} = ½\{[n^2+1+C(n)D\kappa]a_k+[n^2-1-C(n)D\kappa]b_k\exp(-2\kappa h)\} \qquad (11a)$$

$$b_{k+1} = ½\{[n^2-1+C(n)D\kappa]a_k\exp(2\kappa h)+[n^2+1-C(n)D\kappa]b_k\} \qquad (11b)$$

when $D_{k+1}\kappa_{k+1} = D_k\kappa_k = D\kappa$ and $\kappa_{k+1}h_{k+1} = \kappa_k h_k = \kappa h$, where h_k, h_{k+1} are the widths of the kth and (k+1)th layers, enabling the coefficients a_{k+1}, b_{k+1} to be related a_k, b_k. The results for the approximate boundary condition eqn (2) are obtained on setting C(n) = 0 in eqns (11a, b). Successive application of these relations yields the coefficients a_k, b_k for all the layers involved, with appropriate boundary conditions chosen for the first and last [12]. A parallel set of coefficients a_k', b_k', for C(n) = 0, enables direct comparison of the accurate and approximate scalar fluxes φ_k, φ_k' in each layer, and thus evaluation of the cumulative error for the multi-layer system. This is illustrated in Fig 3, with $\Delta\varphi/\varphi = 1.4\%$ at a single interface (for $\varpi_0 = 0.995$, g = 0.95, n = 1.1), the cumulative error increasing with the total number of layers, exceeding 30% for 5 layers when $\kappa_s'/\kappa_a = 1$. For multi-layer media with higher index ratios or larger numbers of layers, the cumulative error can easily exceed 100%.

In conclusion, application of an approximate boundary condition for the diffuse flux at an interface between scattering media of differing refractive index results in an error in the scalar flux φ proportional to the vector flux J, increasing with refractive index ratio n. The fractional error $\Delta\varphi/\varphi = C(n)\langle\mu\rangle$, where $C(n)\propto(n-1)^{3/2}$ for $n-1\ll1$ [1] and $\langle\mu\rangle$ is the mean cosine of the boundary radiance. In media characterised by strongly forward biased scattering, such as biological tissue, the error increases rapidly with absorption (Fig. 1). Reducing the scattering asymmetry by rescaling via the δ-P1 approximation increases the effective absorption, and may offset the reduction in flux error. The error is cumulative in a multi-layer system and can be prohibitive in calculating the diffuse flux distribution. The use of asymptotic plane wave solutions greatly simplifies the analysis; solutions for a point source in a diffusing cylinder can be obtained via a Hankel transform [12].

References

1. R. Aronson, J. Opt. Soc. Am. A **12** 2532-2539 (1995)
2. G. W. Faris, J. Opt. Soc. Am A **19** 519-520 (2002)
3. J. Ripoll, M. Nieto-Vesperinas, J. Opt. Soc. Am. A **16** 1947-1957 (1999)
4. J. S. Cassell, M. M. R Williams, J. Quant. Spect. Rad. Trans. **104** 400-427 (2007)
5. J-M. Tualle, J. Prat, E Tinet, S Avrillier, J. Opt. Soc. Am. A **17** 2046-2055 (2000)
6. M. Shendeleva, J. Opt. Soc. Am. A **27** 1521-1528 (2010)
7. V. I. Haltrin, Appl. Opt. **27** 599-602 (1988)
8. B. Davison *Neutron Transport Theory* (OUP 1957)
9. S. A. Carp, S. A. Prahl, V. Venugopalan, J. Biomed. Opt. **9** 632-647 (2004)
10. D. C. Sahni, E. B. Dahl, N. G. Sjöstrand, Phys. Med. Biol. **48** 3969-3976 (2003)
11. R. Aronson, J. Opt. Soc. Am. A **16** 1066-1071 (1999)
12. A. Liemert, A. Kienle, Opt Express **18** 9266-9279 (2010)
13. W. M. Star, SPIE Inst. Ser. **IS5** 146-154 (1989)
14. E. L. Hull, T. H. Foster, J. Opt. Soc. Am. A **18** 584-599 (2001)
15. L. G. Henyey, J. A. Greenstein, Astrophys. J. **93** 70-83 (1941)

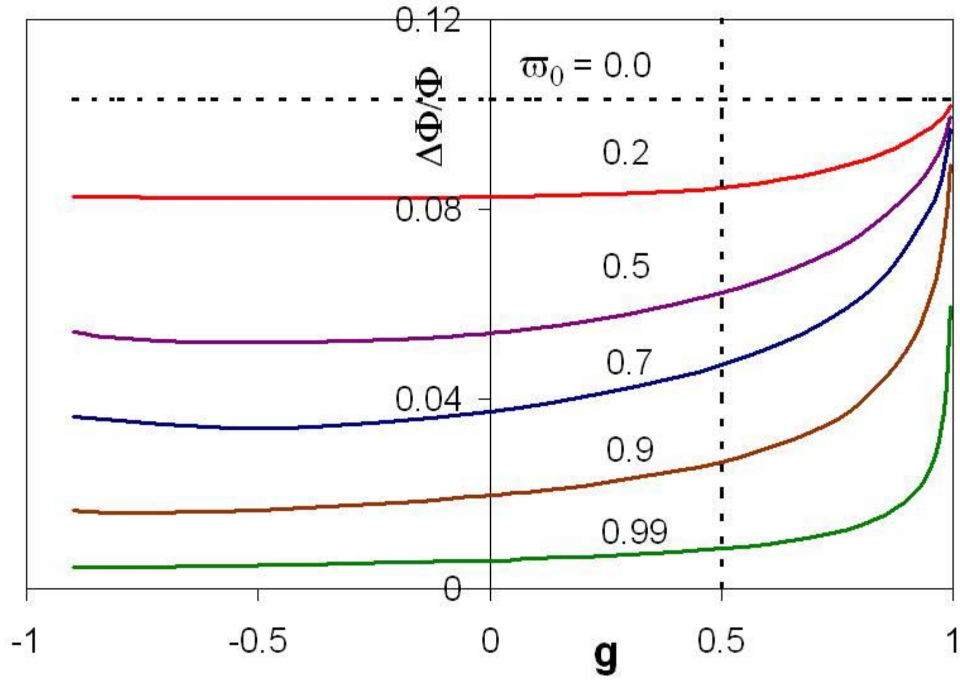

Fig. 1. Relative flux error $\Delta\varphi/\varphi$ vs scattering asymmetry g for a range of scattering albedoes ϖ_0, the error increasing rapidly for g>0.9. The limiting case for zero scattering (ϖ_0 = 0) is indicated by the horizontal dashed line; the vertical dotted line marks the maximum asymmetry in the δ–P1 approximation (g' = 0.5). Index ratio n = 1.06.

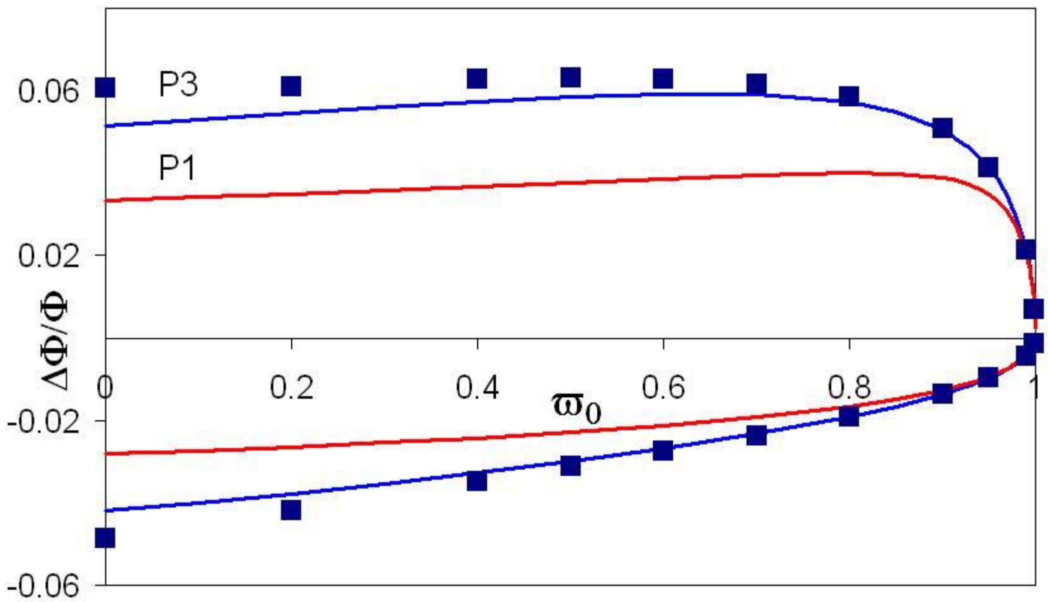

Fig. 2. Relative error in diffuse flux density on either side of the interface between two homogeneous scattering media with disparate scattering parameters: g = 0.95 (upper curves), g = 0 (lower curves) for index ratio n = 1.06. The filled squares (■) are data points calculated with accurate values of the diffusion parameters D, κ [10, 11].

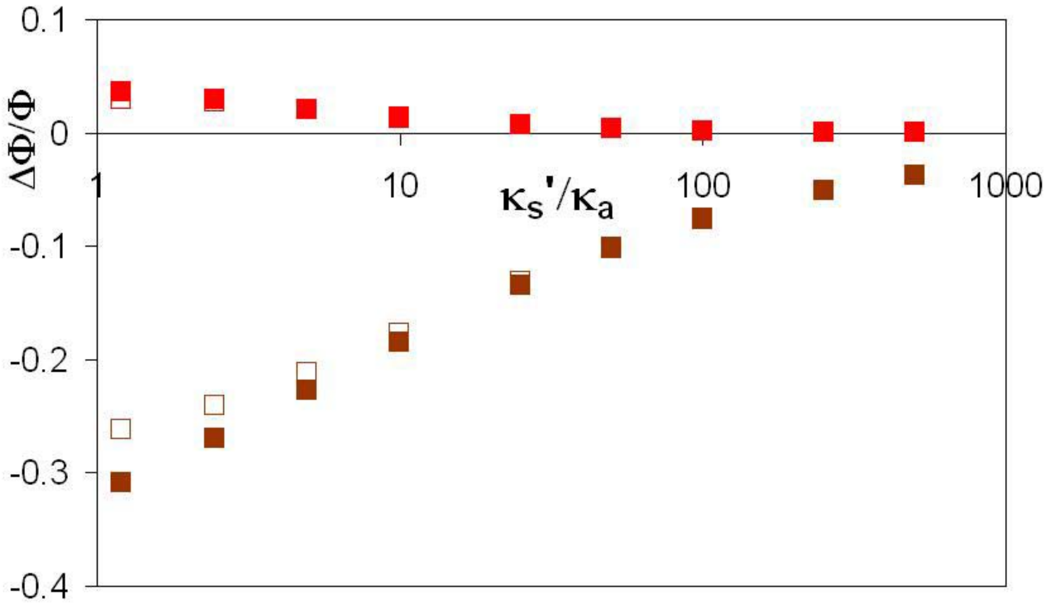

Fig. 3. Relative flux error vs. κ_s'/κ_a in layer 1 (upper points) and layer 5 (lower points) of a 5-layer medium on a half-space (g = 0.95, index ratios n = 1.1); open squares (□) P1 (diffusion) values, filled squares (■) accurate values of diffusion parameters D, κ.