Boundary conditions for diffusion of light

Raphael Aronson

Bioimaging Sciences Corporation, 64 Burnett Terrace, West Orange, New Jersey 07052

Received April 3, 1995; accepted May 31, 1995

In connection with recent work on remote imaging of random media by light, a straightforward generalization of the proper diffusion boundary conditions is presented that takes into account Fresnel reflection. The Milne problem at exterior boundaries is solved for various values of index of refraction, absorption, and scattering anisotropy parameters to yield extrapolated end points and extrapolation distances. A generalized interface condition is derived to replace the usual condition of continuity of intensity. Benchmark-quality numerical results are given for the extrapolation distance and for the new index-dependent parameter in the interface conditions. Difficulties in using the extrapolated end point when the index is sufficiently large are discussed, and a new image procedure suitable for this case is presented.

Key words: diffusion theory, diffusion, light, radiative transfer, diffusion boundary conditions, diffusion interface conditions, extrapolation distance, extrapolated end point, method of images.

1. INTRODUCTION

The past few years have seen considerable and growing interest in the passage of near-infrared light through biological tissue, with a view to developing new diagnostic methods.[1] It is accepted generally in the field that a transport model can be used for analysis and, more particularly, that the diffusion approximation is applicable in most cases of interest. Just as neutron diffusion became a prime tool in the analysis of nuclear reactors, photon diffusion has become a prime tool in this new field of optical diffusion tomography.[2] The essential difference between neutron (or, more generally, particle) diffusion and photon diffusion is that for particles a change in the medium changes only the diffusion properties; for photons there is also reflection when the index of refraction changes. This reflection affects the diffusion solutions by changing the boundary conditions. There have been extensive efforts to derive boundary conditions,[3–8] mostly approximate. Here "exact" results are presented, exact in the sense that we start from the standard prescriptions for boundary conditions for particles, add only the effect of Fresnel reflection, and obtain exact results for the resulting integrals.

The usual procedure is to determine exterior boundary conditions from the solution of the transport equation, to which the diffusion equation is an approximation, while interior boundary conditions (interface conditions) are determined in a sense self-consistently within diffusion theory. For this reason, we will discuss them separately. For the exterior problem we obtain modifications to the universally accepted particle extrapolation distance of 0.7104 mean free path.[9] For the interior problem we obtain a modification of the condition that the intensity is continuous at an interface. The new condition involves a single parameter that depends only on the relative index of refraction. Tables and graphs of this function and also a good parametric fit are given. Finally, we compare our results with approximate results given in the literature. We consider the external problem first.

2. EXTERIOR BOUNDARIES

It is well known that the diffusion equation requires nonphysical exterior boundary conditions for its solution. It is obvious that physically the particle distribution is completely determined by the sources interior to the medium and the incident surface distribution. On the other hand, the diffusion equation is an equation for the intensity, which at a boundary requires knowledge not only of the incident distribution but of the exit distribution as well. Physically this is part of the output, not of the input. In contrast, the exact transport equation requires the physically correct boundary conditions. The problem arises from the fact that diffusion is valid deep in the interior of the medium but not within a boundary region of the order of two or three transport mean free paths. This difficulty is not unique to transport problems. It occurs in a number of fields. For instance, the usual hydrodynamic equations are unsuitable for calculating fluid flow in boundary regions, and a solution of equations valid in the boundary region must be used to determine the appropriate boundary conditions to use for calculations in the bulk.

Which of the infinite number of solutions of the diffusion equation is obtained depends on the boundary conditions chosen. Although diffusion-type boundary conditions are sensibly used at interfaces, they are not appropriate at exterior boundaries because they do not give the correct interior solution. The usual condition used to obtain the correct diffusion solution, i.e., the solution that becomes identical with that for the exact transport equation in the asymptotic region (that is, deep in the interior of the medium), is that the diffusion solution vanish at a certain distance outside the physical boundary. This distance is known as the extrapolated end point.[9] This is generally computed at a free boundary, i.e., one with nothing incident upon it. That is the usual situation considered for light, in which the proximate source of the diffusing light is not the incident light, which is by no means random, but a distribution

0740-3232/95/112532-08$06.00

of scattered light in the interior. The asymptotic intensity satisfies the diffusion equation, and *it* is the solution sought from diffusion theory. It should be stressed that this solution is *not* valid in the boundary region. The extrapolated end point z_0 is defined as the distance from the boundary at which the extrapolated asymptotic intensity curve vanishes; the extrapolation distance d is the distance at which the curve extrapolated linearly from the boundary vanishes. When there is no reflection and no absorption in the medium, the asymptotic intensity curve is linear, and the two are the same. Otherwise the curve is concave, and so long as z_0 exists, $z_0 > d$.

The commonly used extrapolated end point given by transport theory for particles is 0.7104 transport mean free path. This is calculated for a plane boundary from the solution of the Milne problem (sources in the deep interior) for a nonabsorbing medium with isotropic scattering.[9] It is useful because the quantity cz_0, where c is the probability of the particle's surviving a single collision, is exceedingly close to 0.7104 transport mean free path over quite a wide range of absorption[9] and is not even a strong function of the curvature of the boundary surface.[10]

Diffusion of light is different from that for particles in just one significant aspect. Particles do not recognize boundaries. They merely experience different conditions on one side of a boundary from those on the other. On the other hand, light is subject to reflection and refraction at boundaries. Because we are here interested in the effect of a boundary on what goes on within the medium, refraction is not of concern at an exterior boundary, although it is relevant at interfaces. Reflection is important at all boundaries.

Reflection back into the interior occurs in other similar transport problems as well, such as for nuclear reactors, in which the core is generally surrounded by a reflection region to inhibit neutron leakage.[11] In that case, however, the reflector is a physically separate region, so that a two-region diffusion calculation can be done. Here it is merely a boundary with no width. To see the effect of reflection at the exterior boundary, consider the case of total specular reflection. (The reflection of light at a vacuum boundary is specular, though not total.) Every photon reflected from the mirror is the continuation of the path of the mirror image of the incident photon. That is, one can think equally well of the real world with reflection at the mirror or of the real and mirror worlds together, with particles from the mirror world approaching the mirror and going straight through it, while the incident particles from the real world sail right through the mirror, their continuations being the mirror images of the actual particles being reflected from the mirror.

The asymptotic intensity curve is certainly smooth, and because it is even with respect to the mirror surface ($z = 0$), its slope must vanish there. Thus the extrapolation distance is infinite. In the absence of absorption, the asymptotic intensity is linear in z, so that the curve is flat and the extrapolated end point is also infinite. When absorption is present, the extrapolated curve never does reach zero (because it is the mirror image of the real intensity curve, which is everywhere positive), so the extrapolated end point does not exist. In that case the extrapolated asymptotic intensity curve never goes to zero but reaches a minimum and starts increasing with increasing distance from the boundary.

3. ANALYSIS: EXTERIOR BOUNDARIES

The extrapolated end point z_0 is defined as the distance from a vacuum boundary at which the asymptotic part of the solution of the Milne problem vanishes. This is the problem of transport in a half-space $z \geq 0$ with a source infinitely far into the interior. Mathematically, z_0 is defined in plane geometry by the condition

$$I^{\rm as}(-z_0) = 0\,, \tag{1}$$

where $I^{\rm as}(z)$ is the asymptotic intensity at a distance z into the medium. It can be seen that the definition of d in Section 2 is equivalent to

$$d = I^{\rm as}(0)/I^{\rm as\prime}(0)\,, \tag{2}$$

where the prime indicates a derivative with respect to z.

The asymptotic intensity for the Milne problem in a half-space with nonvanishing absorption can be shown to be of the form[9]

$$I^{\rm as}(z) = \exp(\lambda z) + A\exp(-\lambda z)\,, \tag{3}$$

where A is a constant determined by solution of the transport equation. It depends on the properties of the medium and on the reflection at the free surface. It is unity for total reflection and decreases with decreasing reflection to a value in the interval $(-1, 0)$ in the absence of reflection [greater than -1 because $I^{\rm as}(0)$ must be positive and less than 0 because the leakage from the boundary must reduce $I^{\rm as}$].

Equation (3) is clearly a solution of the time-independent diffusion equation $f'' - \lambda^2 f = 0$, so λ has to be identified with the reciprocal of the diffusion length. From the definitions we see that

$$z_0 = -(1/2\lambda)\ln(-A)\,, \tag{4}$$

$$d = \frac{1}{\lambda}\,\frac{1+A}{1-A}\,. \tag{5}$$

These are just two ways of representing the value of the parameter A that determines the asymptotic intensity, so which of these quantities one uses is purely a matter of convenience. When there is no absorption, $\lambda = 0$. An analytic limiting procedure leads to a linear form $I^{\rm as}(z) = z_0 + z$ in place of Eq. (3), with $d = z_0$.

In the presence of absorption, A is positive for sufficiently strong reflection, and z_0 is then complex. Physically this corresponds to the absence of an extrapolated boundary—the extrapolated intensity never vanishes. There are two reasonable possibilities for dealing with this. If one uses the boundary conditions directly, one should prescribe d rather than z_0. But often it is convenient to use the method of images. Aside from an irrelevant scale factor, Eq. (3) can be rewritten as $I^{\rm as}(z) = \sinh\lambda(z + z_0)$ when $A < 0$, so $I^{\rm as}$ plus its extrapolation for negative z is odd about $z = -z_0$. Thus one can account for the effect of the boundary on $I^{\rm as}$ for $z > 0$ by adding to any source S at z' an image source $S' = -S$ at $-2z_0 - z'$. An extension of this idea is suggested here for use when $A > 0$. An extrapolated end point no longer exists, but, again aside from a scale factor, Eq. (3) is equivalent to $I^{\mathrm{as}}(z) = \cosh \lambda(z + z_1)$, where $z_1 = \mathrm{Re}(z_0) = -(1/2\lambda)\ln A$. The extrapolated solution is even about z_1, so the image source corresponding to an actual source S at z' is $S' = +S$ at $-2z_1 - z'$.

I previously used the transfer matrix method to solve the Milne problem with a reflecting boundary condition characterized by the reflection function R.[12,13] The A used here is the $\mathcal{F}_{00}$ of the latter reference, and the λ is called λ_0 there. The resulting expressions for z_0 and d are evaluated here in a double-P_N approximation.[12,14] In this approximation, R is represented by a square matrix $\mathbf{R}$ of order $N + 1$.

In the particle case a plane vacuum boundary is nonreentrant. That is, any particle incident on the boundary escapes and is lost. In that case, $\mathbf{R} = 0$. For light, one must take account of Fresnel reflection at the boundary. To describe the reflection, let μ' be the cosine of the angle of incidence, μ be the cosine of the angle of reflection, μ_0 be the cosine of the angle of refraction into vacuum, μ_c be the cosine of the critical angle, and n be the index of refraction.

Snell's law gives

$$\mu_0^2 = 1 - n^2 + n^2\mu^2. \tag{6}$$

At the boundary there is Fresnel reflection. In the spirit of diffusion theory, which implies randomness in polarization as well as in direction of the light, we must assume unpolarized light incident on the boundary. The reflection coefficient can be written as

$$R(\mu, \mu') = r(\mu)\delta(\mu - \mu'), \tag{7}$$

where the Dirac delta function is the mathematical representation of the fact that the reflection is specular and[15]

$$\begin{aligned} r(\mu) &= \frac{1}{2}\left[\left(\frac{\mu - n\mu_0}{\mu + n\mu_0}\right)^2 + \left(\frac{\mu_0 - n\mu}{\mu_0 + n\mu}\right)^2\right], \qquad \mu \geq \mu_c\,, \\ &= 1, \qquad \mu \leq \mu_c\,. \end{aligned} \tag{8}$$

The quantity $r(\mu)$ gives the reflection probability for a photon incident upon the boundary at an angle $\cos^{-1}\mu$.

In the double-P_N approximation, the elements of $\mathbf{R}$ are given for $0 \leq i, j \leq N$ by[14]

$$\begin{aligned} R_{ij} &= (2i + 1)\int_0^1 D_i(\mu)\mathrm{d}\mu \int_0^1 R(\mu, \mu')D_j(\mu')\mathrm{d}\mu' \\ &= (2i + 1)\int_0^1 r(\mu)D_i(\mu)D_j(\mu)\mathrm{d}\mu \\ &= \delta_{ij} - (2i + 1)s_{ij}\,, \end{aligned} \tag{9}$$

where

$$s_{ij} = \int_{\mu_c}^1 [1 - r(\mu)]D_i(\mu)D_j(\mu)\,\mathrm{d}\mu\,. \tag{10}$$

In these equations δ_{ij} is the Kronecker delta and the $D_i(\mu)$ are the half-range Legendre polynomials:

$$D_i(\mu) = P_i(2\mu - 1)\,. \tag{11}$$

Inasmuch as $D_i(\mu)D_j(\mu)$ is a polynomial in μ, the integrals are sums of terms of the form

$$J_k = \int_{\mu_c}^1 [1 - r(\mu)]\mu^k\,\mathrm{d}\mu\,. \tag{12}$$

One way of proceeding is to use the substitution $t = (n\mu - \mu_0)/\sqrt{n^2 - 1}$, which gives

$$\begin{aligned} J_k = {} & \frac{1 - \mu_c^{k+1}}{k + 1} - \frac{1}{2}\left(\frac{\sqrt{n^2 - 1}}{2n}\right)^{k+1} \\ & \times \int_p^1 \left[t^4 + \left(\frac{t^2 - g}{1 - gt^2}\right)^2\right] \frac{(1 + t^2)^k(1 - t^2)}{t^{k+2}}\,\mathrm{d}t\,, \end{aligned} \tag{13}$$

where $\mu = \sqrt{n^2 - 1}\,(t^2 + 1)/2nt$, $g = (n^2 - 1)/(n^2 + 1)$, and $p = [(n - 1)/(n + 1)]^{1/2}$.

The integrand in Eq. (13) is a rational function of t, so the integral can be evaluated exactly. The resulting expressions are extremely cumbersome, so this approach was used only as a check. For the primary calculations, the integration variable was taken to be $x = 2\mu_0 - 1$. This gives

$$\begin{aligned} s_{ij} = (1/n)\int_{-1}^1 & \left[\frac{1}{(\mu + n\mu_0)^2} + \frac{1}{(\mu_0 + n\mu)^2}\right] \\ & \times D_i(\mu)D_j(\mu)\mu_0^2\mathrm{d}x\,. \end{aligned} \tag{14}$$

Here $\mu_0 = (1 + x)/2$ and, from Eq. (6), $\mu = (n^2 - 1 + \mu_0^2)^{1/2}/n$.

The quantity s_{i0} was evaluated for $0 \leq i \leq 2N$ by a 96-point Gaussian quadrature. One expects this to give good results for N less than ~48. In fact, no difference was found between the values calculated by exact and Gaussian integration for selected R_{i0} for $N = 30$. The integrals were also checked by use of $y = (2t - 1 - p)/(1 - p)$ as the integration variable . The integrals in s_{i0} were transformed to integrals over y from -1 to 1 and a 96-point Gaussian integration applied to these. Because this is an inherently different integration scheme from the integration over x, the results serve as a check on the Gaussian approximation. Again they were found to be accurate.

The s_{ij} for $0 < j \leq i \leq 2N - j$ were calculated from the recursion relation

$$s_{i,j+1} = \frac{1}{j + 1}\left\{\frac{2j + 1}{2i + 1}[(i + 1)s_{i+1,j} + is_{i-1,j}] - js_{i,j-1}\right\}, \tag{15}$$

which follows from the recursion relation for the Legendre polynomials. Because of the symmetry of s_{ij}, this gives all the s_{ij} for $0 \leq i, j \leq N$ and therefore all the required R_{ij}.

4. INTERFACES

Inasmuch as the diffusion equation is a second-order partial differential equation in space, one boundary condition is required at the exterior boundary and two conditions are required at any interior interface between two media. For particle diffusion, the usual conditions are that the intensity and flux be continuous across the interface.[11] Continuity of flux is demanded by the diffusion equation itself, if one integrates it across the narrow interface region. From the physical point of view, the diffusion equation is a continuity equation for the particles. Continuity of flux expresses the same thing—a finite number of particles cannot be absorbed in an infinitesimally small region. For particles, the intensity is taken as continuous across an interface because the diffusing particles do not recognize an interface when they cross it. The collision probabilities change on the other side, but there are no road signs at the interface itself. Photons, by contrast, see a change in the index of refraction, so it cannot be required that the photon intensity be continuous across a material discontinuity.

The procedure of the previous sections can in principle be used at an interface between two media, but it seldom is. Just as at an exterior boundary, one can calculate the extrapolated end point for each medium in the presence of the other, making use of the reflection properties of medium 1 is computing z_0 for medium 2 and vice versa. The drawback of this scheme is twofold. First, the problem at hand resembles the Milne problem only for the medium that contains the sources and only if the sources are in the deep interior. Second, there is no nearly universal number such as 0.71 because the result depends on the combined properties of both media. If they are identical, for instance, z_0 is infinite. In fact, ordinarily two media resemble each other much more than either resembles a vacuum, because a condition for the validity of diffusion theory is that the absorption be small. This means that the effect of internal discontinuities is less severe than that for a free surface.

5. ANALYSIS: PARTICLE DIFFUSION AT INTERFACES

We take as a starting point the well-known formulas for the partial fluxes at an interface, in plane geometry. We take the stratification perpendicular to the z axis and ask for the downward flux J_- across the plane $z = 0$. With the standard diffusion theory assumptions of no absorption, isotropic scattering and weakly varying particle distribution, a first-order expansion in the intensity gives[11]

$$\begin{aligned} J_- &= (\phi/2)\int_0^1 \mu \mathrm{d}\mu + (\phi'/2\,\Sigma_t)\int_0^1 \mu^2 \mathrm{d}\mu \\ &= \phi/4 + \phi'/6\,\Sigma_t\,, \end{aligned} \tag{16}$$

where Σ_t is the macroscopic total cross section, ϕ is the intensity at $z = 0$, and ϕ' is the derivative of ϕ there. Similarly, the upward flux through the plane $z = 0$ is

$$\begin{aligned} J_+ &= (\phi/2)\int_0^1 \mu \mathrm{d}\mu - (\phi'/2\,\Sigma_t)\int_0^1 \mu^2 \mathrm{d}\mu \\ &= \phi/4 - \phi'/6\,\Sigma_t\,. \end{aligned} \tag{17}$$

The net upward flux is

$$J = J_+ - J_-\,. \tag{18}$$

Away from an interface, where ϕ is continuous, this gives

$$J = -(1/3\,\Sigma_t)\phi'. \tag{19}$$

The basic approximation of diffusion is Fick's law:

$$\mathbf{J} = -D\nabla\phi\,. \tag{20}$$

Comparison with Eq. (19) gives

$$D = 1/3\Sigma_t\,. \tag{21}$$

Thus we may rewrite Eqs. (16) and (17) as

$$J_- = (1/4)\phi + (1/2)D\phi' = (1/4)\phi - (1/2)J\,, \tag{22}$$

$$J_+ = (1/4)\phi - (1/2)D\phi' = (1/4)\phi + (1/2)J\,. \tag{23}$$

If there is a material boundary at the interface, so that the cross sections are different on the two sides, then D is discontinuous. As J is continuous, ϕ' is discontinuous.

There are many ways of deriving these results, all of which involve an assumption of weakly varying angular intensity. When the assumptions are relaxed, as when the scattering is slightly anisotropic or there is some absorption, different derivations lead to somewhat different results. For instance, the elementary kinetic theory derivation leads to an additional factor of Σ_s/Σ_t in the presence of absorption, where Σ_s is the macroscopic scattering cross section. A derivation starting from an assumption that the angular intensity is linear in μ does not give this factor. This should not be too surprising. The difference in any computed intensities is of higher order in Σ_s/Σ_t. We choose to work with Eqs. (16) and (17). Further, the main effect of anisotropic scattering is to replace Σ_t in Eqs. (16), (17), and (21) by the transport cross section Σ_{tr}, defined by[11]

$$\Sigma_{\text{tr}} = (1 - g)\Sigma_s + \Sigma_a\,, \tag{24}$$

where Σ_a is the macroscopic absorption cross section and the anisotropy parameter g is the average cosine of the scattering angle. In the following discussion we will assume that this replacement has been made.

6. PHOTON DIFFUSION

Consider a material discontinuity at $z = 0$. Let the diffusion coefficient and the index of refraction be $D_1 = 1/(3\Sigma_{\text{tr}})_1$ and n_1, respectively, for $z > 0$ and $D_2 = 1/(3\Sigma_{\text{tr}})_2$ and n_2 for $z < 0$. The relative index of refraction in going from the upper medium to the lower one is $n = n_2/n_1$. Equations (16) and (17) must both be modified to include a factor $1 - r$ in the integrand. We must also take into account the discontinuity of ϕ at the interface, taking $\phi = \phi_1$ in the expression for J_- and $\phi = \phi_2$ in the expression for J_+.

In all generality we can take $n > 1$. We will define the cosine of the angle of incidence from below as μ and that from above as μ_0. The partial fluxes at the interface are then

$$J_- = \phi_1/2 \int_0^1 [1 - r(\mu_0)]\mu_0 \mathrm{d}\mu_0 + 3D_1\phi_1'/2 \times \int_0^1 [1 - r(\mu_0)]\mu_0^2 \mathrm{d}\mu_0 , \tag{25}$$

$$J_+ = \phi_2/2 \int_0^1 [1 - r(\mu)]\mu \mathrm{d}\mu - 3D_2\phi_2'/2 \times \int_0^1 [1 - r(\mu)]\mu^2 \mathrm{d}\mu . \tag{26}$$

If we think of μ and μ_0 as defining directions in the two media without regard to whether they refer to angle of incidence, angle of reflection, or angle of refraction, then they are related by Snell's law, Eq. (6). Because the net flux J is continuous, Fick's law gives

$$D_1\phi_1' = D_2\phi_2' = -J . \tag{27}$$

Thus

$$J_- = (A_1\phi_1 - B_1 J)/2 , \tag{28}$$

$$J_+ = (A_2\phi_2 + B_2 J)/2 , \tag{29}$$

where

$$A_1 = \int_0^1 [1 - r(\mu_0)]\mu_0 \,\mathrm{d}\mu_0 , \tag{30}$$

$$A_2 = \int_{\mu_c}^1 [1 - r(\mu)]\mu \,\mathrm{d}\mu , \tag{31}$$

$$B_1 = 3\int_0^1 [1 - r(\mu_0)]\mu_0^2 \,\mathrm{d}\mu_0 , \tag{32}$$

$$B_2 = 3\int_{\mu_c}^1 [1 - r(\mu)]\mu^2 \,\mathrm{d}\mu . \tag{33}$$

Subtracting Eq. (28) from Eq. (29) gives

$$J = (A_2\phi_2 - A_1\phi_1)/(2 - B_1 - B_2) . \tag{34}$$

Keijzer *et al.*[3] approximated the reflection coefficient by an exponential function and integrated the resulting expressions for A_1, A_2 and $B_1 + B_2$. An exact result is given here.

7. EXACT INTERFACE CONDITION

It is apparent from Eqs. (6) and (8) that $r(\mu_0, n) = r(\mu, 1/n)$. Here we have explicitly inserted the relative index of refraction into the expression for r. Because from Eq. (6), $\mu_0 \mathrm{d}\mu_0 = n^2\mu\,\mathrm{d}\mu$, we see immediately that $A_1 = n^2 A_2$. This result was previously obtained by Cohen[16] in the case in which there is no net flux, and it is also perhaps implicit in some work of Preisendorfer.[17] We find the result here in complete generality. Then, from Eq. (34),

$$\phi_2 - n^2\phi_1 = C(n)J , \tag{35}$$

where we have explicitly pointed out the n-dependence of C, which is defined by

$$C(n) = (2 - B_1 - B_2)/A_2 . \tag{36}$$

Because B_1 and B_2 are both less than unity and A_2 is positive, $C(n)$ is also positive.

Now B_1 and B_2 are computed just like the J_1 and J_2 defined in Eq. (12). Further, the same argument that relates A_1 and A_2 gives

$$B_1 = 3\int_{\mu_c}^1 [1 - r(\mu)]\mu_0\mu \,\mathrm{d}\mu . \tag{37}$$

In terms of the integration variable t discussed in Section 3 one has $\mu_0 = \sqrt{n^2 - 1}(1 - t^2)/2t$. The integrand is again a rational function of t, similar to that for B_2. Thus the integrals in A_2, B_2, and B_1 can all be carried out analytically when they are transformed into integrals over t. The resulting formulas are given in Appendix A. The analytical result for A_1 was known to Walsh[18] in somewhat different form as early as 1926.

As in Section 3, here we used a 96-point Gaussian integration over the variable $x = 2\mu_0 - 1$ defined before Eq. (14). As before, agreement between those results and the analytical ones was essentially perfect.

At a free boundary, $J = J_+$, and Eqs. (2), (27), and (29), along with $D_2 = 1/3\Sigma_{tr}$, give the expression $d = (2 - B_2)/3A_2$ as an alternative to the extrapolation distance calculated from transport theory. We will see some numerical results for this expression, but, as discussed above, this approach has little physical justification.

8. RESULTS

The quantities d and z_0 have been computed as functions of n and the single-scattering albedo $c = \Sigma_s/\Sigma_t$. Most of the results were for isotropic scattering, but some calculations for anisotropic scattering were also carried out. The double-P_N calculations used $N = 30$, but convergence was excellent even for $N = 5$, for which z_0 was computed correctly to four decimal places. All the results are given in units of the mean free path.

Table 1 gives values of cz_0, which is less dependent on c than is z_0, for $1 < n < 2$ and for $1.00 > c > 0.90$ for isotropic scattering. The results are shown graphically in Fig. 1 for $c = 1$ and $n < 5$ and in Fig. 2 for $c < 1$ and $n < 2$. For $c = 1$, $d = z_0$. The values of cz_0 for $c < 1$ are seen to rise remarkably rapidly with n, the more so as the absorption increases. For instance, for no absorption and $n = 1.5$, cz_0 is more than triple the value of 0.71 for $n = 1$. For 5% absorption, it is more than four times as large. For $n \geq 2.1$, z_0 is not real for $c \leq 0.99$. In Fig. 2, each curve for $c \leq 0.98$ ends. This means that z_0 goes

Table 1. Extrapolated End Point Times c, Isotropic Scattering

	c							
n	1.00	0.99	0.98	0.97	0.96	0.94	0.92	0.90
1.0	0.71	0.71	0.71	0.71	0.71	0.71	0.71	0.71
1.1	0.88	0.88	0.88	0.87	0.87	0.86	0.86	0.85
1.2	1.15	1.14	1.14	1.13	1.13	1.12	1.11	1.10
1.3	1.47	1.48	1.48	1.48	1.48	1.48	1.48	1.48
1.4	1.86	1.88	1.90	1.93	1.96	2.02	2.09	2.19
1.5	2.30	2.37	2.44	2.54	2.65	3.00	3.84	—
1.6	2.79	2.95	3.16	3.46	3.97	—	—	—
1.7	3.32	3.66	4.21	5.52	—	—	—	—
1.8	3.92	4.58	6.32	—	—	—	—	—
1.9	4.56	5.87	—	—	—	—	—	—
2.0	5.25	8.11	—	—	—	—	—	—

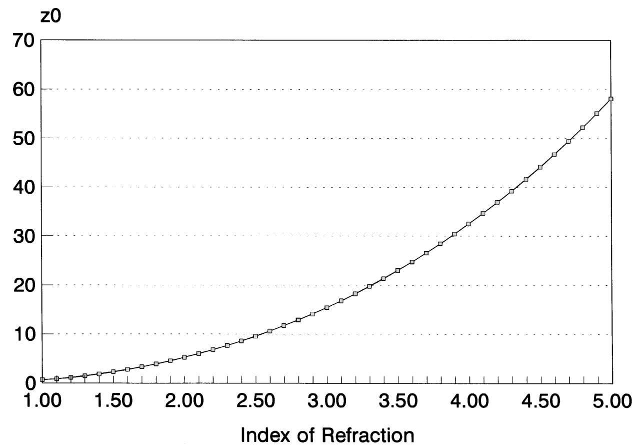

Fig. 1. Extrapolated end point. No absorption, isotropic scattering.

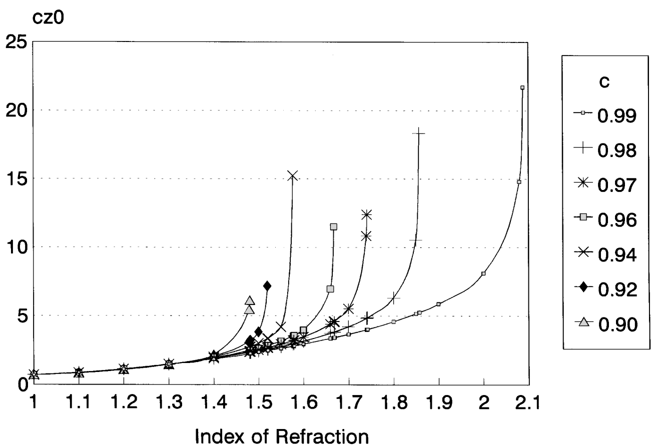

Fig. 2. Extrapolated end point times c. Isotropic scattering.

to infinity before the next data point. By contrast, the extrapolation distance d, shown in Table 2 and Fig. 3 for the same range of c and $n \leq 3$, is well behaved for all values of the index of refraction. Like z_0, d increases rapidly with n. It also decreases with c. Appendix B gives quartic fits to d for several values of c for $1 < n < 3$.

Table 2 and Fig. 3 also show, for comparison, the diffusion-based result $d = (2 - B_2)/3A_2$ discussed in Section 7. The result is not bad for $c = 1$, but it deteriorates as the absorption increases. This is not surprising, because it is derived for $c = 1$ and does not contain c as a parameter. In contrast to a Milne problem calculation, it cannot take into account any anisotropy, either.

To show the effect of anisotropy, d was calculated both for linearly anisotropic scattering and for a Henyey–Greenstein phase function. Table 3 shows $(1 - gc)d$ for an anisotropy parameter $g = 0.8$, along with the comparable values for isotropic scattering. The factor $1 - gc$ is just Σ_{tr} in our units, so this table gives d in units of the transport mean free path. In these units, linear anisotropy has remarkably little effect even for this large anisotropy factor, and even the more-peaked Henyey–Greenstein anisotropy does not make a large difference.

For the interface problem the quantity $C(n)$ is tabulated in Table 4 and shown graphically in Fig. 4. It is zero, as expected, when $n = 1$. The results for $1 < n < 3.73$ were fitted in two separate ranges, with an error of less than 4% at worst. The independent variable is taken to be $p = [(n - 1)/(n + 1)]^{1/2}$, and $p_1 = p - 0.64$. The result is

Table 2. Extrapolation Distance, Isotropic Scattering

	c						
n	1.00	0.98	0.96	0.94	0.92	0.90	Diffusion
1.0	0.71	0.72	0.72	0.73	0.74	0.75	0.67
1.1	0.88	0.88	0.88	0.88	0.88	0.88	0.90
1.2	1.15	1.13	1.12	1.10	1.09	1.08	1.20
1.3	1.47	1.44	1.41	1.39	1.36	1.33	1.56
1.4	1.86	1.81	1.76	1.72	1.67	1.63	1.97
1.5	2.30	2.23	2.16	2.09	2.03	1.97	2.42
1.6	2.79	2.69	2.60	2.52	2.43	2.35	2.92
1.7	3.32	3.21	3.09	2.98	2.87	2.77	3.47
1.8	3.92	3.77	3.63	3.49	3.36	3.23	4.07
1.9	4.56	4.38	4.21	4.05	3.89	3.73	4.72
2.0	5.25	5.05	4.85	4.65	4.46	4.27	5.42
2.1	6.00	5.76	5.53	5.30	5.07	4.85	6.17
2.2	6.81	6.53	6.26	5.99	5.73	5.48	6.98
2.3	7.67	7.35	7.04	6.74	6.44	6.15	7.84
2.4	8.59	8.23	7.88	7.53	7.19	6.86	8.77
2.5	9.57	9.16	8.77	8.38	8.00	7.62	9.75
2.6	10.61	10.16	9.71	9.28	8.85	8.43	10.79
2.7	11.71	11.21	10.71	10.23	9.75	9.29	11.90
2.8	12.88	12.32	11.78	11.24	10.71	10.19	13.07
2.9	14.11	13.50	12.90	12.30	11.72	11.15	14.30
3.0	15.42	14.74	14.08	13.43	12.79	12.16	15.61

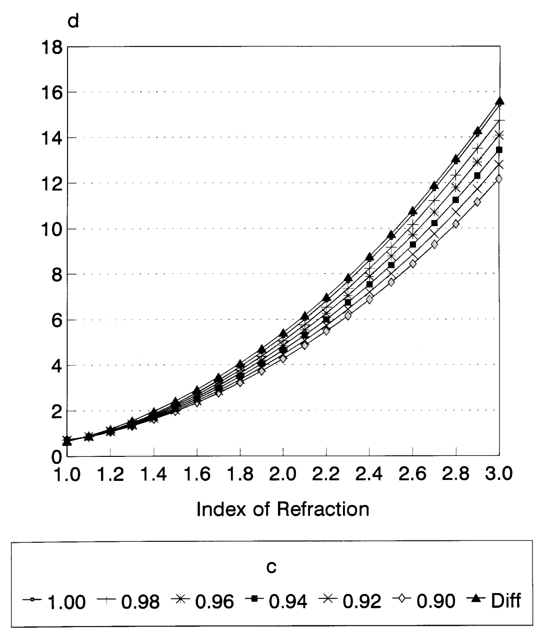

Fig. 3. Extrapolation distance. Isotropic scattering, transport mean free path units.

Table 3. Extrapolation Distance, $g = 0.8$, in Transport Mean Free Paths[a]

	$c = 1.0$			$c = 0.9$		
n	Iso	Lin	H–G	Iso	Lin	H–G
1.3	1.47	1.47	1.47	1.33	1.36	1.23
2.0	5.25	5.25	5.34	4.27	4.45	3.59
3.0	15.42	15.42	16.10	12.16	12.66	9.90

[a]Iso, isotropic; Lin, linear; H–G, Henyey–Greenstein.

Table 4. Interface Coefficient $C(n)$

n	$C(n)$	n	$C(n)$
1.0	0.00	2.2	10.97
1.2	0.66	2.4	14.46
1.4	1.86	2.6	18.51
1.6	3.47	2.8	23.16
1.8	5.51	3.0	28.44
2.0	7.99		

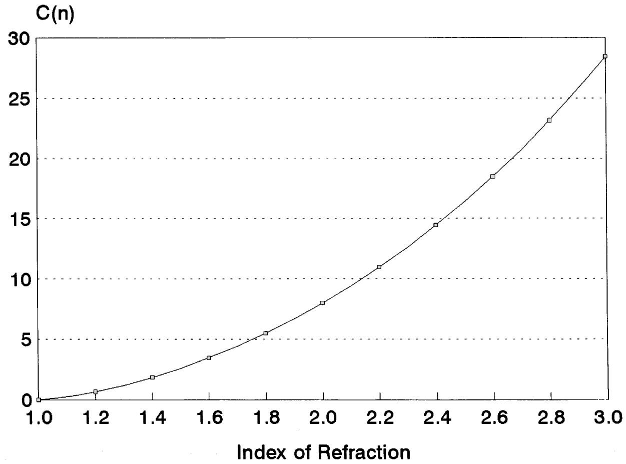

Fig. 4. Interface coefficient $C(n)$.

$$C(n) = 25.6p^3[1 - (45/32)p + (83/21)p^2], \quad 1 < n < 1.82,$$
$$= 14.3(1 + 9.35p_1 + 49.1{p_1}^2 + 327{p_1}^3 + 1800{p_1}^4), \quad 1.82 \leq n \leq 3.73. \quad (38)$$

The form for $n < 1.82$ is just the small-p expansion of $C(n)$. The form for larger n is a quartic fit to the data.

9. DISCUSSION

This paper has presented conditions at both interior and exterior boundaries that should be used to describe the diffusion of light. At an exterior boundary, a description in terms of the extrapolation distance d is more suitable than one in terms of the extrapolated end point z_0 because d is positive for all finite n. Alternatively, a new variation of the method of images has been suggested here for use when z_0 is complex, in which a source S at z' is supplemented with an image source $S' = +S$ at $-2z_1 - z'$, where $z_1 = \mathrm{Re}(z_0)$. The effect of reflection is to increase z_0 and d greatly. The error in neglecting extrapolation is therefore much greater than for particles. If one wishes to neglect the effect in a particular application, it is necessary to justify the neglect. If extrapolation is taken into account, it is not appropriate to use the extrapolation distance of 0.71 transport mean free path used for particles. Rather, the data given here should be used. Although diffusion-based values of d have been presented here for comparison, I cannot think of any possible reason for using them. The transport theory results are here and available. The only way that one could be confident in using the diffusion approach is *post hoc,* since one has to do a transport theory calculation anyway to justify the diffusion-type results. As expected, the diffusion-type results become closer and closer to the transport theory results with no absorption as the reflection increases. This is to be expected—the effect of the discontinuity becomes smaller and smaller.

The consistent diffusion interface condition for photons has been used to derive Eq. (35), and exact results for the coefficient $C(n)$ of the flux have been presented. The results do not depend on the cross sections of the two materials.

One final caveat remains: These conditions, like the corresponding conditions for particle diffusion, were obtained by consideration of problems with plane symmetry. The motivation for this and related studies comes typically from situations in which the diffusion sources are line sources, so that there is also a relevant radial variable. That is, the results are being applied to situations for which they were never meant. This is not much of a difficulty for the interface conditions, because the media for the most part are large, and the lateral dimensions of their interfaces cover many mean free paths. The problem is for exterior boundary conditions. A partial justification is that nothing better is available. But also, radiation at boundary points far from the source has for the most part traveled through regions well into the interior,[19,20] and so the situation somewhat resembles the Milne problem. It is expected, then, that the exterior boundary conditions obtained here should hold fairly well far from the source. Near the source, they do not, but this is precisely the region in which the diffusion solution cannot be expected to be very good anyway.

APPENDIX A: INTERFACE CONSTANTS

The results of the integrations for A_1, B_1, and B_2 are

$$A_1 = \frac{5n^6 + 8n^5 + 6n^4 - 5n^3 - n - 1}{3(n^2+1)^2(n^2-1)(n+1)} - \frac{4n^4(n^4+1)}{(n^2+1)^3(n^2-1)^2}\log n + \frac{n^2(n^2-1)^2}{2(n^2+1)^3}\log\frac{n+1}{n-1}, \quad (A1)$$

$$B_1 = 1 - \frac{3(n^2-1)^{3/2}}{16}(I_0 - I_1 - I_2 + I_3), \quad (A2)$$

$$B_2 = 1 - \frac{(n^2-1)^{3/2}}{n^3}\left[1 + \frac{3}{16}(I_0 + I_1 - I_2 - I_3)\right], \quad (A3)$$

where

$$I_n = (1 - p^{2n+1})/(2n+1) + J_n, \quad (A4)$$

$$J_0 = \frac{16n^4}{(n^2+1)^4}K_2 - \frac{8n^2(n^2-1)^2}{(n^2+1)^4}K_1 - \frac{8n^2(n^2-1)}{(n^2+1)^3} \times \left(\frac{1}{p} - 1\right) + \frac{(n^2-1)^2}{3(n^2+1)^2}\left(\frac{1}{p^3} - 1\right), \quad (A5)$$

$$J_1 = \frac{16n^4}{(n^2+1)^3(n^2-1)}K_2 - \frac{8n^2(n^4+1)}{(n^2+1)^3(n^2-1)}K_1 + \frac{(n^2-1)^2}{(n^2+1)^2}\left(\frac{1}{p} - 1\right), \quad (A6)$$

$$J_2 = \frac{16n^4}{(n^2+1)^2(n^2-1)^2} K_2 - \frac{8n^2}{(n^2+1)^3(n^2-1)} K_1 + \frac{(n^2+1)^2}{(n^2-1)^2}(1-p), \quad \text{(A7)}$$

$$J_3 = \frac{16n^4}{(n^2+1)(n^2-1)^3} K_2 - \frac{8n^2(n^4+4n^2+1)}{(n^2+1)(n^2-1)^3} K_1 + \frac{8n^2(n^2+1)}{(n^2-1)^3}(1-p) + \frac{(n^2+1)^2}{3(n^2-1)^2}(1-p^3), \quad \text{(A8)}$$

$$K_1 = \sqrt{\frac{n^2+1}{n^2-1}} \left(\log \frac{\sqrt{n^2+1}+\sqrt{n^2-1}}{\sqrt{n^2+1}+n-1} + \frac{1}{2}\log n \right), \quad \text{(A9)}$$

$$K_2 = \frac{n^2+1}{4}\left(1-\frac{p}{n}\right) + \frac{1}{2}K_1, \quad \text{(A10)}$$

$$p = \sqrt{\frac{n-1}{n+1}}. \quad \text{(A11)}$$

APPENDIX B: FIT TO EXTRAPOLATION DISTANCE

The following quartic fits to d for isotropic scattering for various values of c in the range from 1.0 to 0.9 are accurate to within 3% in the range $1 < n < 3$:

$$\begin{aligned} d &= 2.94 - 7.01n + 5.76n^2 - 1.16n^3 + 0.159n^4, \quad c = 1.00 \\ &= 2.98 - 6.96n + 5.68n^2 - 1.16n^3 + 0.157n^4, \quad c = 0.98 \\ &= 2.83 - 6.50n + 5.30n^2 - 1.06n^3 + 0.144n^4, \quad c = 0.96 \\ &= 2.63 - 5.94n + 4.84n^2 - 0.94n^3 + 0.129n^4, \quad c = 0.94 \\ &= 2.77 - 6.16n + 5.00n^2 - 1.03n^3 + 0.139n^4, \quad c = 0.92 \\ &= 2.79 - 6.10n + 4.95n^2 - 1.04n^3 + 0.140n^4, \quad c = 0.90. \end{aligned} \quad \text{(B1)}$$

ACKNOWLEDGMENTS

The author's interest in the effect of a discontinuous index of refraction on diffusion boundary conditions was stimulated by a conversation with Norman McCormick. The encouragement of Randall Barbour is also acknowledged. Thanks are due to Scott Prahl for pointing out Refs. 17 and 18 and to Gerald Pomraning for a helpful discussion. The author thanks Harry Graber for reading the manuscript critically. This research was supported in part by the National Institutes of Health under grant RO1 CA59955, by the New York State Science and Technology Foundation, and by the U.S. Office of Naval Research under grant N000149510063.

REFERENCES AND NOTES

1. See, for instance, R. L. Barbour, H. L. Graber, Y. Wang, and R. Aronson, "A perturbation approach for optical diffusion tomography using continuous-wave and time-resolved data," in *Medical Optical Imaging: Functional Imaging and Monitoring,* G. Müller *et al.,* eds., Vol. IS11 of Institute Series (SPIE, Bellingham, Wash., 1993), pp. 87–120.
2. For an overview of much current work, see A. Yodh and B. Chance, "Spectroscopy and imaging with diffusing light," Phys. Today **48**(3), 34–40 (1995).
3. M. Keijzer, W. M. Star, and P. R. M. Storchi, "Optical diffusion in layered media," Appl. Opt. **27,** 1820–1824 (1988).
4. J. X. Zhu, D. J. Pine, and D. A. Weitz, "Internal reflection of diffusive light in random media," Phys. Rev. A **44,** 3948–3959 (1991).
5. I. Freund, "Surface reflections and boundary conditions for diffusive photon transport," Phys. Rev. A **45,** 8854–8858 (1992).
6. R. Aronson, "Exact interface conditions for photon diffusion," in *Physiological Monitoring and Early Detection Diagnostic Methods,* T. Mang, ed., Proc. Soc. Photo-Opt. Instrum. Eng. **1641,** 72–78 (1992).
7. R. Aronson, "Extrapolation distance for diffusion of light," in *Photon Migration and Imaging in Random Media and Tissues,* B. Chance and R. R. Alfano, eds., Proc. Soc. Photo-Opt. Instrum. Eng. **1888,** 297–305 (1993).
8. For a comparative study of various proposed boundary conditions, see R. C. Haskell, L. O. Svaasand, T.-T. Tsay, T.-C. Feng, M. S. McAdams, and B. J. Tromberg, "Boundary conditions for the diffusion equation in radiative transfer," J. Opt. Soc. Am. A **11,** 2727–2741 (1994).
9. K. M. Case and P. F. Zweifel, *Linear Transport Theory* (Addison-Wesley, Reading, Mass., 1967).
10. R. Aronson, "Subcritical problems in spherical geometry," Nucl. Sci. Eng. **86,** 436–449 (1984).
11. See, for instance, J. R. Lamarsh, *Introduction to Nuclear Reactor Theory* (Addison-Wesley, Reading, Mass., 1983), Chap. 5.
12. R. Aronson, "Transfer matrix solution of some one- and two-medium transport problems in slab geometry," J. Math. Phys. **11,** 931–940 (1970).
13. R. Aronson, "Traveling mode solution of transport-theory problems by inspection," Transp. Theory Stat. Phys. **2,** 181–196 (1972).
14. G. Caroll and R. Aronson, "One-speed neutron transport problems. Part II: Slab transmission and reflection and finite reflector critical problems," Nucl. Sci. Eng. **51,** 166–179 (1973).
15. M. Born and E. Wolf, *Principles of Optics,* 2nd ed. (Pergamon, New York, 1964).
16. A. Cohen, "Photoelectric determination of the relative oxygenation of blood," Ph.D. dissertation (Carnegie-Mellon University, Pittsburgh, Pa., 1969).
17. R. W. Preisendorfer, *Hydrologic Optics* (U.S. Department of Commerce, National Oceanic and Atmospheric Administration, Washington, D.C., 1976), Section 2.6.
18. Unpublished report by Walsh quoted by J. W. Ryde, "The scattering of light by turbid media," Proc. R. Soc. London Ser. A **131,** 451–475 (1931).
19. R. F. Bonner, R. Nossal, S. Havlin, and G. H. Weiss, "Model for photon migration in turbid biological media," J. Opt. Soc. Am. A **4,** 423–432 (1987).
20. R. L. Barbour, H. L. Graber, R. Aronson, and J. Lubowsky, "Imaging of subsurface regions of random media by remote sensing," in *Time-Resolved Spectroscopy and Imaging of Tissues*, B. Chance, ed., Proc. Soc. Photo-Opt. Instrum. Eng. **1431,** 192–203 (1993).