Diffusion boundary conditions for photon waves

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ABSTRACT

The use of diffusion theory in calculations on photon waves necessitates a new look at boundary conditions, since the standard boundary conditions have been derived under static conditions. When the underlying process satisfies the transport equation, the proper boundary conditions are obtained by solving the Milne problem. This paper presents benchmark-quality values for extrapolation distances calculated by transport theory, for various values of absorption and three models of the phase function—isotropic, linearly anisotropic and Henyey-Greenstein scattering. The results show that the static boundary conditions are perfectly adequate up to photon wave frequencies of 1 GHz or even more. Specifically, the quantity $\Sigma_{tr}d$, where $\Sigma'_{tr} = \Sigma_{tr} - ik$, where Σ_{tr} is the macroscopic transport cross section and k the wave number in the medium and d the linear extrapolation distance, is essentially independent of frequency over this range. We have also examined the ratio of the diffusion length as given by transport theory to that given by diffusion theory itself. This is extremely insensitive to frequency, but for substantial absorption, using the diffusion theory result can lead to substantial errors in thick media, especially for Henyey-Greenstein scattering.

Keywords: diffusion, transport theory, Milne problem, diffusion boundary conditions, photon waves

1. INTRODUCTION

In recent years there has been an ever-increasing amount of work, employing photon waves, on imaging abnormalities in tissue,[1-7] using both simulation and experiment. The corresponding mathematical analysis required for image reconstruction usually uses diffusion theory.

In a recent paper[8] I discussed the problem of the proper diffusion boundary conditions for calculations of diffusion of light, both at interfaces and at external boundaries. These, and so far as I know, all previous calculations of boundary conditions[7] have been done for time-independent situations. The question posed and answered here is how the static boundary conditions must be modified to take account of photon waves. Secondarily, this paper discusses the error in the usual diffusion length formula for the diffusion length in terms of the diffusion coefficient and the absorption cross section.

For any given problem the diffusion solution involves two constants, since the diffusion equation is a second-order differential equation. One constant can be thought of as a scale parameter, determined by the magnitude of the source. The second is a shape parameter, giving the form of the solution. This parameter is generally determined by either the extrapolated end point z_0 or the linear extrapolation distance d. Simply put, the extrapolated end point is the distance outside the physical boundary at which the asymptotic intensity curve extrapolates to zero. The extrapolation distance is the distance outside the physical boundary at which a linear extrapolation with the slope given by that at the boundary vanishes. These two quantities are related to each other; each can be computed from the other. In the absence of reflection or absorption, the asymptotic intensity curve is linear, and $z_0 = d$. Contrary to many statements in the literature, in any problem for a thick medium for which mixed (Type III) boundary conditions can be used successfully for diffusion calculations, Dirichlet (Type I) conditions can be used as well, so long as the extrapolated end point is real, and they give the same answers. Which one uses is a matter of convenience, not of necessity.

It is assumed here that the underlying process is governed by the transport equation, which assumes well-defined collisions with free travel for the photons in between. This condition is certainly not satisfied in tissue. Nevertheless, it is generally accepted by people working in the field that the independent collision picture described by transport theory is at least basically correct. Certainly the success people have had in imaging using that model gives some support to assuming that it is basically valid. In any case, there is no accepted rationale for determining the boundary conditions otherwise. Transport theory says that the appropriate constants to use are those given by the Milne problem.

Reference 6 gives values for the extrapolated end point and/or the extrapolation distance for various values of the index of refraction obtained by an exact (that is, converged) transport solution of the Milne problem, taking into account Fresnel reflection at the boundary. The present work extends these results to photon waves. From a technical point of view, this merely requires solving the Milne problem with reflective boundary conditions using complex rather than real arithmetic, and the resulting values of d and z_0 are complex.

2. ANALYSIS

The time-dependent diffusion equation in a uniform medium is

$$\frac{1}{v}\frac{\partial I(\mathbf{r},t)}{\partial t} - D\nabla^2 I(\mathbf{r},t) + \Sigma_a I(\mathbf{r},t) = S(\mathbf{r},t). \tag{1}$$

Here $I(\mathbf{r},t)$ is the intensity at position vector $\mathbf{r}$ and time t, $S(\mathbf{r},t)$ is the source strength at $\mathbf{r}$ and t, D is the diffusion coefficient, Σ_a the macroscopic absorption cross section and v the speed of light in the medium. For a density wave of angular frequency ω, one can write

$$I(\mathbf{r},t) = \phi(\mathbf{r})e^{-i\omega t}. \tag{2}$$

Inserting this into the diffusion equation gives

$$D\nabla^2\phi(\mathbf{r},t) - \Sigma'_a\phi(\mathbf{r},t) = -S(\mathbf{r},t), \tag{3}$$

where

$$\Sigma'_a = \Sigma_a - ik. \tag{4}$$

Here k is the wave number in the medium:

$$k = \omega/v = 2\pi fn/c_0, \tag{5}$$

where f is the modulation frequency, c_0 is the speed of light in vacuum and n is the index of refraction.

The time-dependent transport equation is

$$\frac{1}{v}\frac{\partial I(\mathbf{r},\hat{\Omega},t)}{\partial t} + \hat{\Omega}\cdot\nabla I(\mathbf{r},\hat{\Omega},t) + \Sigma_t I(\mathbf{r},\hat{\Omega},t) = \int d\hat{\Omega}_1 \Sigma_s(\hat{\Omega}_1 \to \hat{\Omega}) I(\mathbf{r},\hat{\Omega}_1,t) + S(\mathbf{r},\hat{\Omega},t). \tag{6}$$

Here $\hat{\Omega}$ is a unit vector in the direction of motion of the photon, Σ_t is the total macroscopic cross section and $\Sigma_s(\hat{\Omega}_1 \to \hat{\Omega})$ is the macroscopic differential scattering cross section from direction $\hat{\Omega}_1$ to direction $\hat{\Omega}$. For a photon wave,

$$I(\mathbf{r},\hat{\Omega},t) = \phi(\mathbf{r},\hat{\Omega})e^{-i\omega t}. \tag{7}$$

Putting this into the transport equation gives the time-independent equation

$$\hat{\Omega}\cdot\nabla\phi(\mathbf{r},\hat{\Omega}) + \Sigma'_t\phi(\mathbf{r},\hat{\Omega}) = \int d\hat{\Omega}_1 \Sigma_s(\hat{\Omega}_1 \to \hat{\Omega})\phi(\mathbf{r},\hat{\Omega}_1) + S(\mathbf{r},\hat{\Omega}), \tag{8}$$

where

$$\Sigma'_t = \Sigma_t - ik = \Sigma_s + \Sigma'_a. \tag{9}$$

Since the scattering cross section doesn't change, the effect is to make absorption cross section complex, just as in diffusion. Note that in a similar way one can define a complex macroscopic transport cross section Σ'_{tr} in terms of the ordinary transport cross section Σ_{tr}:

$$\Sigma'_{tr} = \Sigma_{tr} - ik. \tag{10}$$

It follows that the calculation is identical with the static calculation, except that the analysis and arithmetic are complex, and obviously the results as well. The only fine point from a technical point of view is in deciding which mode corresponds to diffusion. In the double-P_N angular expansion used here, the solution is a sum of spatial exponentials. One looks for the most slowly attenuating mode. In the usual time-independent calculation, the diffusion mode is the one with the largest (real, in that case) reciprocal attenuation constant, which corresponds to the diffusion length. Here, the reciprocal diffusion length is identified with the attenuation constant with the smallest real part.

One relevant parameter is the ratio of k to Σ_t (or, alternatively, the ratio of Σ'_a to Σ_t), just as in the static case it is the ratio of Σ_a to Σ_t. Physically, this is 2π times the number of wavelengths in one mean free path. If this number is not small, the fundamental assumption for the validity of diffusion theory, that the variation in the intensity over a mean free path is small, is violated. In that case, diffusion theory is not valid, and the determination of the correct boundary conditions is then beside the point. For a typical index of refraction of 1.4 for tissue, a frequency of 1 GHz and a mean free path of 1 mm, this ratio is

$$\frac{k}{\Sigma_t} = \frac{2\pi fn}{c_0}\lambda_t = \frac{2\pi \times 1.4 \times 10^9}{3\times 10^8}\times 10^{-3} \approx 0.03 \,. \tag{11}$$

If the dominant dependence on frequency is given entirely by this ratio, one can conclude that for any practical frequency the effect is negligible. If fact, this turns out to be the case, but it was not evident *a priori* that the ratio k/Σ_a was not also involved.

The most common way of showing the result is to give the extrapolated end point. This has the advantage that the combination $\Sigma_{tr}z_0$ (the extrapolated end point in units of the transport mean free path) is extraordinarily insensitive to absorption, if the absorption is small, to the details of the phase function, and even to curvature of the surface. But the presence of index mismatch makes it less suitable for photon transport. The Fresnel reflection cuts down the flux leakage from the surface, making the intensity curve flatter and increasing z_0. It increases quite rapidly with increasing index, and if the reflection is great enough, the extrapolated intensity curve never does vanish, and the extrapolated end point becomes complex, even at zero frequency. The extrapolation distance is always real at zero frequency and even at nonzero frequency its imaginary part remains much smaller than that of z_0. In addition, it varies less with the index of refraction, so d becomes easier to work with than z_0.

3. RESULTS

Tables 1-4 give results for $\Sigma'_{tr}d$, the linear extrapolation distance expressed in units of the complex transport cross section, for frequencies up to 1 GHz, which is in the range in which experiments in diffusion tomography are beginning to be done,[9] and for a transport mean free path of 1 mm. (All the results hold for values of the transport mean free path other than 1 mm so long as the ratio k/Σ_{tr} is held constant. Note that because of the dependence of k on the index of refraction, this is not quite the same as keeping the ratio f/Σ_{tr} constant.) The results are presented in this way because even though d itself depends only very weakly on frequency, the tabulated results depend on frequency even more weakly. The tables are classified by the single-scattering albedo $c = \Sigma_s/\Sigma_t$ and give results for isotropic, linearly anisotropic and Henyey-Greenstein phase functions, the latter two for average cosine g of the scattering angle. Observe that a fixed transport mean free path means that the *total* mean free path for anisotropic scattering is different from that for isotropic scattering and depends on g. The results are given for index for refraction $n = 1.0$, 1.4 (reasonable for tissue) and 2.0, the last to show the effect for a large index. Table 1 is for $c = 1.0$, $g = 0.9$; Table 2 for $c = 1.0$, $g = 0.6$; Table 3 for $c = 0.9$, $g = 0.9$; and Table 4 for $c = 0.9$, $g = 0.6$. That is, the absorption ranges up to 10 per cent and the results cover a large range of anisotropy.

The transport calculations were done in a double- P_N representation by the Transfer Matrix method.[10-12] The results presented are exact to the accuracy shown, and were obtained for $N = 20$ (a 42-stream calculation), but almost all the results even for N=5 agreed with these except for a few that differed by a unit or two in the last place. The computation on a 166-MHz Pentium computer took approximately 0.1 seconds per problem.

The conclusion from the data shown is that the real part of the extrapolation distance is sensibly independent of frequency over the range shown. The imaginary part is linear in frequency and small, less than about 0.02 over the entire range covered, for an index of 1.4. The fact that the imaginary part of $\Sigma'_{tr}d$ is considerably larger for isotropic scattering than for the anisotropic scattering with a large value of g is a result of scaling and was to be expected. For a given value of Σ_{tr}, the total cross section is much smaller for isotropic scattering, and the ratio k/Σ_t is correspondingly larger. For $c = 1.0$, $g = 0.9$, it is larger by a factor of ten.

These results actually hold quite well for isotropic and linear scattering up to about 5 GHz and even beyond. For Henyey-Greenstein scattering, the imaginary part of $\Sigma'_{tr}d$ remains quite linear up to about 5 GHz, but the real part starts to drop somewhat after about 3 GHz. For instance, for c = 1.0, g = 0.9, $\Sigma'_{tr}d$ = 1.871 + 0.085i at 3 GHz and 1.855 + 0.139i at 5 GHz, as compared to the zero-frequency result $\Sigma'_{tr}d$ = 1.880.

4. TRANSPORT CORRECTIONS TO DIFFUSION LENGTH

The inverse attenuation length of the asymptotic mode is given by exact transport theory as $\kappa_0 = \sqrt{3\Sigma_{tr}\Sigma_a}$ at zero frequency to lowest order in the absorption cross section, and is here generalized to $\kappa_0 = \sqrt{3\Sigma'_{tr}\Sigma'_a}$. This mode satisfies a diffusion equation and is identified with the diffusion solution. This result is also given by the P_1- approximation to the transport equation, which gives a diffusion equation. It is also consistent with the diffusion theory result $\kappa_{diff} = \sqrt{\Sigma'_a / D}$, with the diffusion coefficient given by $D = 1/3\Sigma'_{tr}$. As c moves away from 1.0 and k from 0, the transport theory result differs more and more from this expression. In effect transport theory says to modify the expression for the diffusion length (and therefore for the diffusion coefficient) if absorption is substantial. The result depends only on the scattering and absorption properties of the medium, and is independent of any index mismatch.

Consider the ratio of the inverse diffusion length as given by transport theory to the limiting form above. The real part of this ratio is again essentially independent of frequency and the imaginary part is linear, with a value of 0.006 or less at 1 GHz for all the cases examined. Thus let us consider the real part alone. This is unity when c = 1 (no absorption). Table 5 gives the result for c = 0.9 and g = 0.9, 0.8 and 0.6. The limiting form given above is quite good, but the ratio, while small, appears in an exponent and can be very important in thick media.

The numerical results are interesting. The ratio is 1.042 for isotropic scattering, and it is scarcely different for linear anisotropy, independent of g in both cases. The ratio for Henyey-Greenstein scattering is considerably larger, and depends strongly on g. The numerical results for isotropic scattering agree with the expansion given in the classic work of Case, de Hoffmann and Placzek[13]:

$$\frac{\kappa}{\kappa_0} = 1 - \frac{2}{5}(1-c) - \frac{12}{175}(1-c)^2 - \frac{2}{125}(1-c)^3 + \frac{166}{67,375}(1-c)^4 + \dots . \qquad (12)$$

Our ratio is the reciprocal of this. These results hold also in the frequency-dependent case, where the quantity (1 - c) becomes $(\Sigma_a - ik)/(\Sigma_t - ik)$. Similar expansions have not been computed for anisotropic scattering.

5. SUMMARY

In summary:

1. The linear extrapolation distance d, though not necessarily the extrapolated end point z_0, is sensibly independent of frequency for frequencies up to several hundred MHz. The quantity $\Sigma'_{tr}d$ is even more insensitive to frequency. The small frequency dependence of the imaginary part is linear up to about 3 GHz at least.
2. The diffusion length as computed from the diffusion formula is somewhat in error when $\Sigma'_a \neq 0$. This error is only a few per cent for isotropic and linearly anisotropic scattering, but is quite a bit larger for a Henyey-Greenstein phase function. In any case, since it appears in an exponent multiplying a large number in thick media, it is a cause for some concern.

ACKNOWLEDGEMENTS

This work was supported in part by the National Institutes of Health under grants RO1 CA59955 and RO1 CA66184.

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Table 1. $\Sigma'_{tr}d$ for c = 1.0, g = 0.9, Σ_{tr} = 10 cm^{-1}

Index	Freq	Isotropic	Linear	H-G
1.00	0	.710 +.000i	.710 +.000i	.714 +.000i
	200	.710 -.004i	.710 +.000i	.714 -.001i
	600	.710 -.013i	.710 -.001i	.714 -.002i
	1000	.710 -.022i	.710 -.002i	.714 -.004i
1.40	0	1.860 +.000i	1.860 +.000i	1.880 +.000i
	200	1.860 +.004i	1.860 +.000i	1.880 +.004i
	600	1.860 +.012i	1.860 +.000i	1.879 +.012i
	1000	1.860 +.020i	1.860 +.001i	1.879 +.020i
2.00	0	5.252 +.000i	5.252 +.000i	5.290 +.000i
	200	5.252 +.028i	5.252 +.002i	5.290 +.020i
	600	5.252 +.084i	5.252 +.007i	5.289 +.059i
	1000	5.252 +.139i	5.252 +.011i	5.287 +.099i

Table 2. $\Sigma'_{tr}d$ for c = 1.0, g = 0.6, Σ_{tr} = 10 cm^{-1}

Index	Freq	Isotropic	Linear	H-G
1.00	0	.710 +.000i	.710 +.000i	.712 +.000i
	200	.710 -.004i	.710 -.002i	.712 -.002i
	600	.710 -.013i	.710 -.005i	.712 -.006i
	1000	.710 -.022i	.710 -.008i	.713 -.009i
1.40	0	1.860 +.000i	1.860 +.000i	1.871 +.000i
	200	1.860 +.004i	1.860 +.001i	1.871 +.003i
	600	1.860 +.012i	1.860 +.003i	1.871 +.010i
	1000	1.860 +.020i	1.860 +.005i	1.871 +.016i
2.00	0	5.252 +.000i	5.252 +.000i	5.275 +.000i
	200	5.252 +.028i	5.252 +.010i	5.275 +.019i
	600	5.252 +.084i	5.252 +.029i	5.274 +.058i
	1000	5.252 +.139i	5.251 +.049i	5.272 +.097i

Table 3. $\Sigma'_{tr}d$ for c = 0.9, g = 0.9, Σ_{tr} = 10 cm^{-1}

Index	Freq	Isotropic	Linear	H-G
1.00	0	.747 +.000i	.730 +.000i	.783 +.000i
	200	.747 -.005i	.730 -.001i	.783 -.001i
	600	.747 -.014i	.730 -.002i	.783 -.003i
	1000	.747 -.023i	.730 -.003i	.783 -.005i
1.40	0	1.628 +.000i	1.686 +.000i	1.312 +.000i
	200	1.628 +.002i	1.686 +.000i	1.312 +.001i
	600	1.628 +.007i	1.686 +.000i	1.312 +.003i
	1000	1.628 +.012i	1.686 +.000i	1.312 +.006i
2.00	0	4.267 +.000i	4.466 +.000i	3.006 +.000i
	200	4.267 +.022i	4.466 +.002i	3.006 +.006i
	600	4.267 +.067i	4.466 +.007i	3.006 +.018i
	1000	4.267 +.111i	4.466 +.012i	3.006 +.029i

Table 4. $\Sigma'_{tr}d$ for c = 0.9, g = 0.6, Σ_{tr} = 10 cm^{-1}

Index	Freq	Isotropic	Linear	H-G
1.00	0	.747 +.000i	.735 +.000i	.749 +.000i
	200	.747 -.005i	.735 -.002i	.749 -.002i
	600	.747 -.014i	.735 -.005i	.749 -.006i
	1000	.747 -.023i	.735 -.009i	.749 -.010i
1.40	0	1.628 +.000i	1.668 +.000i	1.586 +.000i
	200	1.628 +.002i	1.668 +.000i	1.586 +.002i
	600	1.628 +.007i	1.668 +.001i	1.586 +.005i
	1000	1.628 +.012i	1.667 +.002i	1.586 +.008i
2.00	0	4.267 +.000i	4.406 +.000i	4.065 +.000i
	200	4.267 +.022i	4.406 +.007i	4.064 +.011i
	600	4.267 +.067i	4.405 +.021i	4.064 +.033i
	1000	4.267 +.111i	4.405 +.035i	4.063 +.055i

Table 5. Ratio of Asymptotic Attenuation Length to Diffusion Value

g	Isotropic	Linear	H-G
0.6	1.042	1.041	1.061
0.8	1.042	1.040	1.098
0.9	1.042	1.040	1.157