Extrapolation distance for diffusion of light

Raphael Aronson

Department of Physics, Polytechnic University
Brooklyn, NY 11021

ABSTRACT

Diffusion theory has been a useful and frequently applied analytical method to study the transport of light in random media. The diffusion equation requires unphysical boundary conditions. This is reflected in the fact that the diffusion solution must differ from the exact solution in a boundary region a few mean free paths thick. Exact transport theory indicates that for particle diffusion the true boundary is to be replaced by an extrapolated boundary 0.71 transport mean free paths outside of it. This is the number that has universally been used in treating light diffusion, although it is sometimes neglected because it is often a very short distance. However, because there is reflection at the boundary due to a mismatch in the index of refraction, the extrapolation distance for diffusion of light is longer than that for particles, and this must be taken into account. The correction is large, even for modest indices of refraction. We show here that the appropriate boundary condition is given in terms of an extrapolation distance and tabulate this quantity as a function of relative scattering probability and index of refraction of the medium.

1 INTRODUCTION

Modeling the transport of light in random media by a diffusion approximation has long been a useful tool for analysis. Diffusion of light requires different boundary conditions from diffusion of particles because of the reflection that occurs at a change in the index of refraction. We have recently given results for the appropriate conditions at interfaces between two regions[1].

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 a 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. 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[2]. This is generally computed at a free boundary, *i.e.*, one with nothing incident on 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 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. Figure 1 shows schematically the total intensity and the asymptotic (diffusion) intensity near a plane surface. The extrapolated end point z_0 is 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. In the case shown in Figure 1, $z_0 > d$.

The commonly used extrapolated end point given by transport theory for particles is 0.71 transport mean free paths. 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. It is useful because the quantity cz_0, where c is the probability the particle surviving a single collision, is exceedingly close to 0.71 transport mean free paths over quite a wide range of absorption[2], differential cross section[2] and curvature of the boundary surface[3].

Diffusion of light is different than that for particles in just one significant aspect. Particles do not recognize boundaries. They merely experience different conditions on one side of a boundary than they do on the other. On the other hand, light is subject to reflection and refraction at boundaries. Since we are here interested in the effect of an exterior boundary on what goes on within the medium, the refraction is not of concern in this work. The reflection is important, however.

Reflection 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[4]. 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 is certainly continuous, and since it is even with respect to the mirror surface ($x = 0$), its slope must vanish there. Thus the extrapolation distance is infinite. In the absence of absorption, the asymptotic intensity is linear in x, 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 general, the slope at the boundary decreases with increasing reflection, and thus with increasing index of refraction. The situation with substantial reflection is shown schematically in Figure 2. In contrast to the case in Figure 1, the asymptotic intensity curve never goes to zero, but reaches a minimun and starts increasing with increasing distance from the boundary. Somewhere between the two cases, z_0 increases to infinity and then becomes meaningless, while d increases with increasing reflection but does not become infinite except in the case of perfect reflection.

2 ANALYSIS

The extrapolated end point 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 for a half-space $x \geq 0$ with a source infinitely far into the interior. Mathematically, z_0 is defined in plane geometry by the condition

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

where $I^{as}(x)$ is the asymptotic intensity at a distance x into the medium. It can be seen that the definition of d in the previous section is equivalent to

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

where the prime indicates a derivative with respect to x.

The asymptotic intensity for the Milne problem in a half-space can be shown to be of the form[2]

$$I^{as}(x) = e^{\lambda x} + Ae^{-\lambda x}, \tag{3}$$

where A is a constant determined by solving the transport equation. It depends on the properties of the medium and on the reflection at the free surface. This is clearly a solution of the time-independent diffusion equation

$$f'' - \lambda^2 f = 0, \tag{4}$$

so λ has to be identified with the reciprocal of the diffusion length. From the definitions we see that

$$z_0 = -(1/2\lambda)\ln(-A) \tag{5}$$

$$d = \frac{1}{\lambda}\frac{A+1}{1-A}. \tag{6}$$

Since these are just two alternative ways of representing the value of the parameter A that determines the asymptotic intensity, which of these quantities one uses is purely a matter of convenience. Note, however, that z_0 is not real when $A > 0$, while d is well-defined for all $A < 1$. $A = 1$ corresponds to perfect reflection, and A decreases with decreasing reflection. Positive values of A correspond to the absence of an extrapolated boundary. It follows that in the presence of reflection, it is appropriate to characterize the boundary conditions by prescribing d rather than z_0.

We have solved the problem using the Transfer Matrix method[5] in a double-P_N approximation[2]. Our A is the $\mathcal{F}_{00}$ of Reference 5 and our λ is λ_0 in that paper. It is shown there that λ is obtained as the smallest positive eigenvalue of a certain matric involving only the properties of the medium and the order N of the approximation. A is the matrix element of a matrix $\mathcal{F}$ both of whose indices correspond to the mode associated with λ. This matrix can be written

$$\mathcal{F} = -(\mathbf{B}_+ - \mathbf{R}\mathbf{B}_-)^{-1}(\mathbf{B}_- - \mathbf{R}\mathbf{B}_+), \tag{7}$$

where the matrices $\mathbf{B}_+$ and $\mathbf{B}_-$ are associated with the eigenvectors of the eigenvalue equation and $\mathbf{R}$ is the reflection matrix for the boundary.

In the particle case a vacuum boundary is nonreentrant. That is, any particle incident on the boundary escapes and is lost. In that case, $\mathbf{R}=\mathbf{0}$. For light, there is Fresnel reflection at the boundary. In the spirit of diffusion theory, which implies randomness in polarization as well as direction of the light, we must assume unpolarized light incident on the boundary. To describe the reflection, let

μ' = cosine of angle of incidence
μ = cosine of angle of reflection
μ_0 = cosine of angle of refraction into vacuum
μ_c = cosine of critical angle
n = index of refraction.

Snell's Law gives

$$\mu_0^2 = 1 - n^2 + n^2\mu^2. \tag{8}$$

The reflection coefficient can be written

$$R(\mu, \mu') = r(\mu)\delta(\mu - \mu'), \tag{9}$$

where the Dirac delta-function is the mathematical representation of the fact that the reflection is specular and[6]

$$r(\mu) = \frac{1}{2}\left[\left(\frac{\mu - n\mu_0}{\mu + n\mu_0}\right)^2 + \left(\frac{\mu_0 - n\mu}{\mu_0 + n\mu}\right)^2\right], \quad \mu \geq \mu_c \tag{10}$$

$$= 1, \quad \mu \leq \mu_c. \tag{11}$$

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

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

$$\begin{aligned} R_{ij} &= (2i+1)\int_0^1 r(\mu)D_i(\mu)D_j(\mu)\,d\mu & (12)\\ &= \delta_{ij} - (2i+1)s_{ij}, & (13)\end{aligned}$$

where

$$s_{ij} = \int_{\mu_c}^1 [1-r(\mu)]D_i(\mu)D_j(\mu)\,d\mu. \tag{14}$$

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

$$D_i(\mu) = P_i(2\mu - 1). \tag{15}$$

It follows that $D_i(\mu)D_j(\mu)$ is a polynomial in μ, so the integrals are sums of terms of the form

$$J_k = \int_{\mu_c}^1 [1-r(\mu)]\mu^k\,d\mu. \tag{16}$$

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

$$J_k = \frac{1-\mu_c^{k+1}}{k+1} - \frac{1}{2}\left(\frac{\sqrt{n^2-1}}{2n}\right)^{k+1}\int_p^1 \left[t^4 + \left(\frac{t^2-g}{1-gt^2}\right)^2\right]\frac{(1+t^2)^k(1-t^2)}{t^{k+2}}\,dt, \tag{17}$$

where

$$\begin{aligned} \mu &= \sqrt{n^2-1}\,(t^2+1)/(2nt), & (18)\\ g &= (n^2-1)/(n^2+1) & (19)\\ p &= \sqrt{(n-1)/(n+1)}. & (20)\end{aligned}$$

The integrand in Eq. (17) is a rational function of t so the integral can be evaluated exactly. The resulting expressions are extremely cumbersome, so we used this approach only as a check. For the primary calculations, the integration variable was taken to be $x = 2\mu_0 - 1$. This gives

$$s_{ij} = (1/n)\int_{-1}^1 \left[\frac{1}{(\mu+n\mu_0)^2} + \frac{1}{(\mu_0+n\mu)^2}\right] D_i(\mu)D_j(\mu)\mu_0^2\,dx. \tag{21}$$

Here $\mu_0 = (1+x)/2$ and, from Eq. (8), $\mu = \sqrt{n^2-1+\mu_0^2}/n$.

We evaluated s_{i0} for $0 \leq i \leq 2N$ by a 96-point Gaussian quadrature. One expects this to give good results for N less than about 48. In fact, we used $N = 30$ and could find no difference for selected R_{i0} between the results of exact and Gaussian integration. The integrals were also checked by using as the integration variable $y = (2t-1-p)/(1-p)$, where t and p are the quantities defined above. The integrals in s_{i0} were transformed to integrals over y from -1 to 1 and a 96-point Gaussian integration applied to these. Since 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

$$s_{i,j+1} = \frac{1}{j+1}\left\{\frac{2j+1}{2i+1}\left[(i+1)s_{i+1,j} + is_{i-1,j}\right] - js_{i,j-1}\right\}, \tag{22}$$

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}.

3 RESULTS

The actual calculations were carried out for $N = 30$. In fact, convergence was excellent even for $N = 5$, for which z_0 was computed correctly to four decimal places. The program was constructed to handle anisotropic as well as isotropic scattering, but all the results presented here are for isotropic scattering.

Table 1 gives values of cz_0 as a function of index of refraction for various scattering probabilities c between 1.00 and 0.90. All distances are in units of the mean free path. For $n \geq 2.1$, z_0 doesn't exist for $c \leq 0.99$. For $c = 1$, the results are identical to those in the first column of Table 2. The results in Table 1 are shown graphically in Figure 3 for $c = 1$ and in Figure 4 for $c < 1$. The values of cz_0 are seen to rise remarkable 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 per cent absorption, it is more than four times as large. The rapid growth of z_0 when the index of refraction approaches the critical index at which z_0 becomes infinite is quite striking in Figure 4.

The extrapolation distance d, by contrast, is well-behaved for all values of the index of refraction. Table 2 and Figure 5 give d as a function of n for various values of c. It can be clearly seen that this is much better behaved as a function of n than is cz_0. Like z_0, d increases rapidly with n.

4 CONCLUSIONS

We have given here boundary conditions at an exterior boundary that should be used to describe the diffusion of light. 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 finite for all finite n. The effect of reflection is to increase these quantities 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 paths used for particles. Rather, the data given here should be used.

5 ACKNOWLEDGEMENTS

The author wishes to thank Gerald Pomraning for a helpful discussion about the results.

6 REFERENCES

1. R. Aronson, "Exact interface conditions for photon diffusion" *SPIE Proceedings on Physiological Monitoring and Early Detection Diagnostics*, Vol. 1641, pp. 72-78, 1992.

2. K. M. Case and P. F. Zweifel, Linear Transport Theory, Addison-Wesley, Reading, MA, 1967.

3. R. Aronson, "Subcritical Problems in Spherical Geometry", *Nucl. Sci. Eng.* 86, pp. 436-449, 1984.

4. J. R. Lamarsh, Introduction to Nuclear Engineering, Second Edition, Addison-Wesley, Reading, MA, 1975.

5. R. Aronson, "Transfer Matrix Solution of Some One- and Two-Medium Transport Problems in Slab Geometry", *J. Math. Phys.* 11, 931-940, 1970.

6. M. Born and E. Wolf, Principles of Optics, Second Revised Edition, pp. 40-42, Pergamon Press, Oxford, 1964.

Table 1. Extrapolated End Point Times 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	—	—	—	—	—	—

Table 2. Extrapolation Distance

n	1.00	0.99	0.98	0.97	0.96	0.94	0.92	0.90
1.0	0.71	0.71	0.72	0.72	0.72	0.73	0.74	0.75
1.1	0.88	0.88	0.88	0.88	0.88	0.88	0.88	0.88
1.2	1.15	1.14	1.13	1.12	1.12	1.10	1.09	1.08
1.3	1.47	1.46	1.44	1.43	1.41	1.39	1.36	1.33
1.4	1.86	1.84	1.81	1.79	1.76	1.72	1.67	1.63
1.5	2.30	2.26	2.23	2.19	2.16	2.09	2.03	1.97
1.6	2.79	2.74	2.69	2.65	2.60	2.52	2.43	2.35
1.7	3.32	3.27	3.21	3.15	3.09	2.98	2.87	2.77
1.8	3.92	3.84	3.77	3.70	3.63	3.49	3.36	3.23
1.9	4.56	4.47	4.38	4.30	4.21	4.05	3.89	3.73
2.0	5.25	5.15	5.05	4.95	4.85	4.65	4.46	4.27
2.1	6.00	5.88	5.76	5.64	5.53	5.30	5.07	4.85
2.2	6.81	6.67	6.53	6.39	6.26	5.99	5.73	5.48
2.3	7.67	7.51	7.35	7.20	7.04	6.74	6.44	6.15
2.4	8.59	8.41	8.23	8.05	7.88	7.53	7.19	6.86
2.5	9.57	9.36	9.16	8.96	8.77	8.38	8.00	7.62
2.6	10.61	10.38	10.16	9.93	9.71	9.28	8.85	8.43
2.7	11.71	11.46	11.21	10.96	10.71	10.23	9.75	9.29
2.8	12.88	12.60	12.32	12.05	11.78	11.24	10.71	10.19
2.9	14.11	13.81	13.50	13.20	12.90	12.30	11.72	11.15
3.0	15.42	15.08	14.74	14.41	14.08	13.43	12.79	12.16

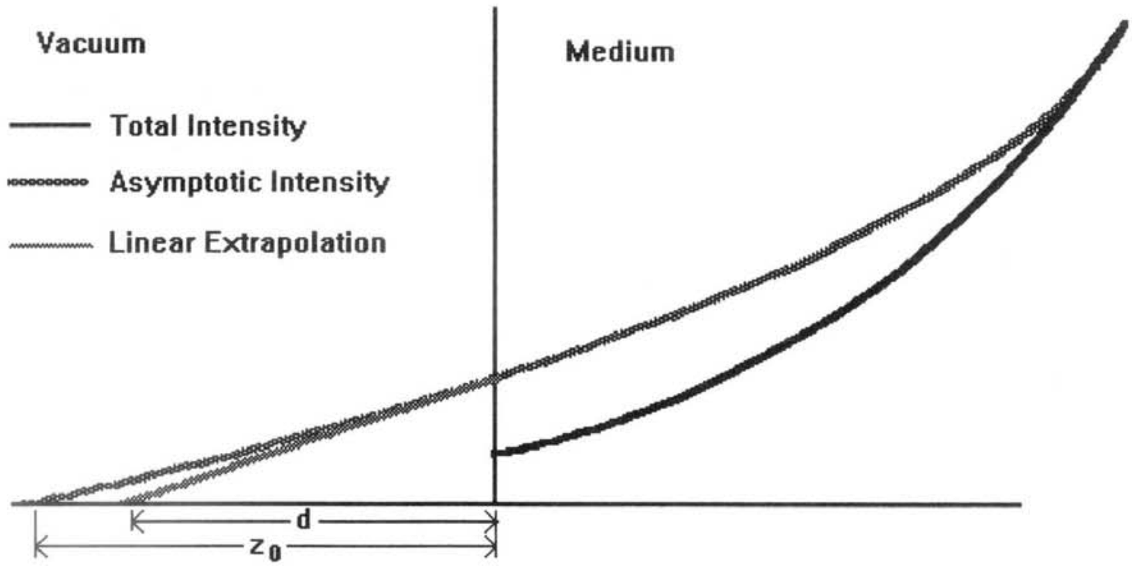

Figure 1. Intensity, No Reflection

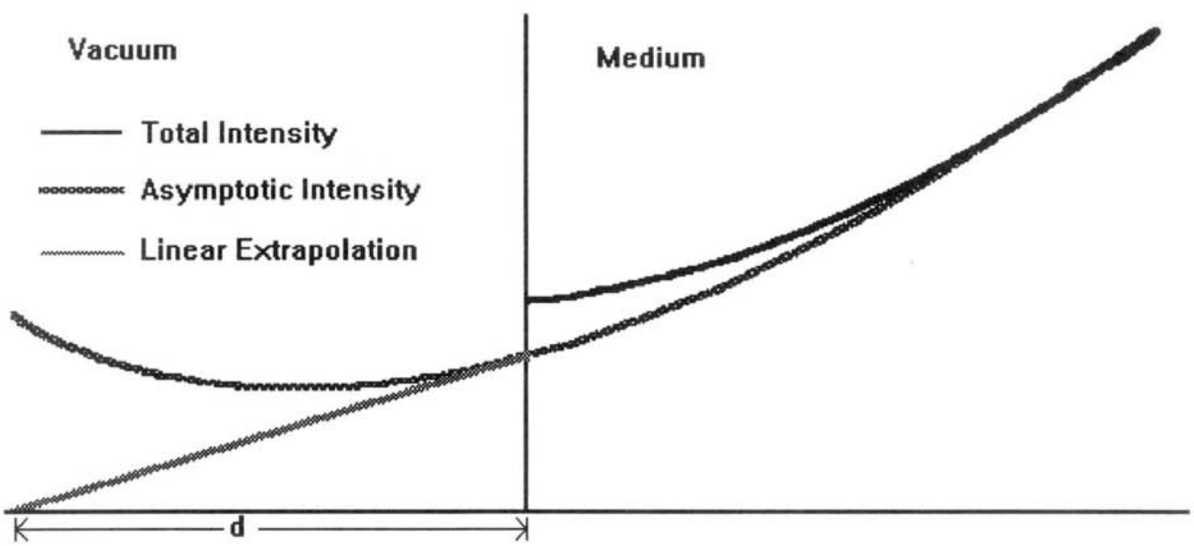

Figure 2. Intensity, Large Reflection

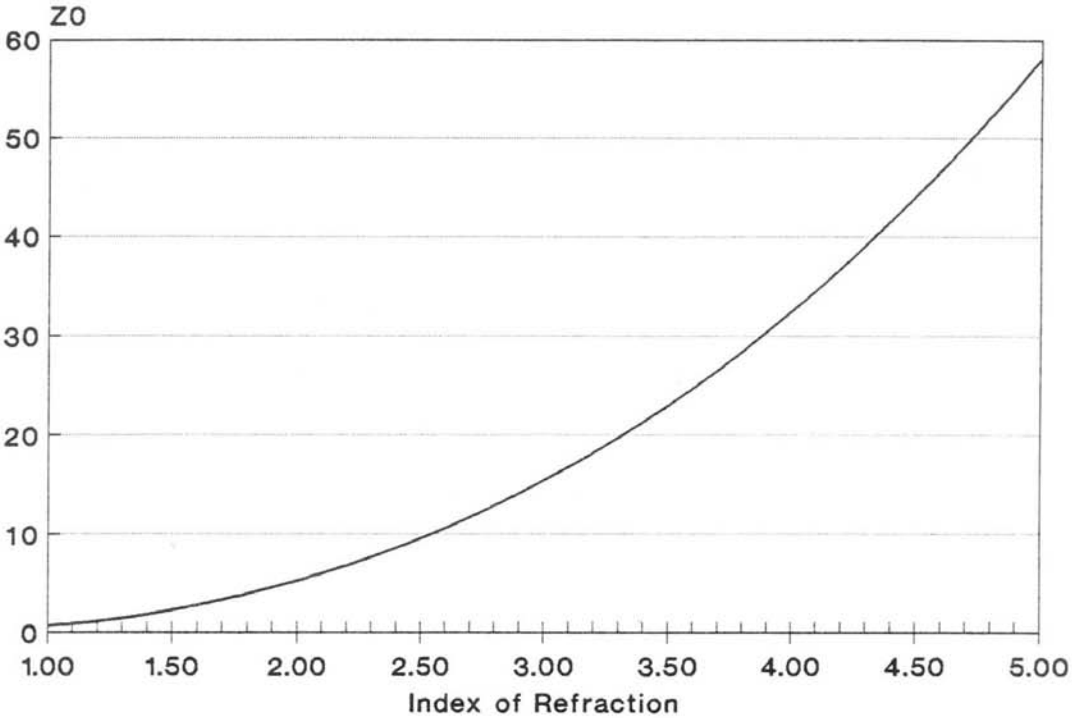

Fig. 3. Extrapolated End Point, No Absorption

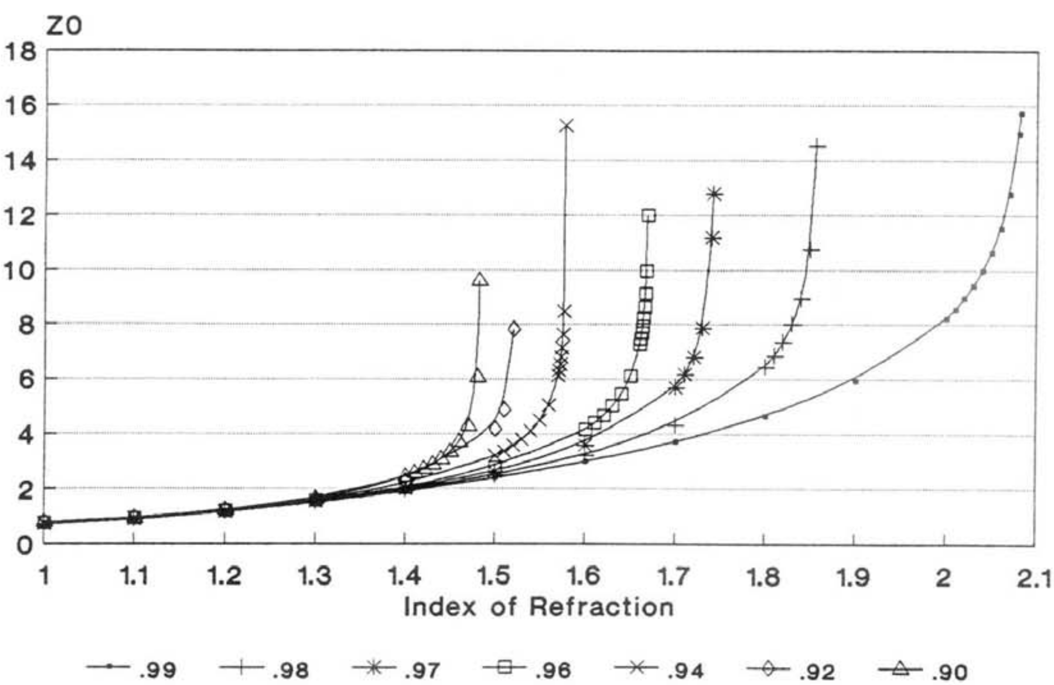

Fig. 4. Extrapolated End Point for Various c

Fig. 5. Extrapolation Distance